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[X] 113 Sheets of Drawings

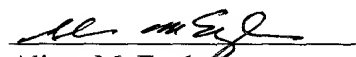
[X] This application claims priority to: a US Provisional application 60/138,308 filed June 9, 1999.

[] Sequence Listing. Provided herein are a formatted Sequence Listing and a copy of the Sequence Listing on computer readable form as required by 37 CFR 1.821 through 1.825

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Respectfully submitted,


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Enclosure

006090-626550

ENGINEERING β -KETOACYL ACP SYNTHASE FOR NOVEL SUBSTRATE SPECIFICITY

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INTRODUCTION

This application claims the benefit of U.S. Provisional Application Number 60/138,308 filed June 9, 1999.

10 Technical Field

The present invention is directed to proteins, nucleic acid sequences and constructs, and methods related thereto.

Background

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Fatty acids are organic acids having a hydrocarbon chain of from about 4 to 24 carbons. Many different kinds of fatty acids are known which differ from each other in chain length, and in the presence, number and position of double bonds. In cells, fatty acids typically exist in covalently bound forms, the carboxyl portion being referred to as a fatty acyl group. The chain length and degree of saturation of these molecules is often depicted by the formula CX:Y, where "X" indicates number of carbons and "Y" indicates number of double bonds.

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The production of fatty acids in plants begins in the plastid with the reaction between acetyl-CoA and malonyl-ACP to produce acetoacetyl-ACP catalyzed by the enzyme, β -ketoacyl-ACP synthase III. Elongation of acetyl-ACP to 16- and 18- carbon fatty acids involves the following cycle of reactions: condensation with a two-carbon unit from malonyl-ACP to form a β -ketoacyl-ACP (β -ketoacyl-ACP synthase), reduction of the keto-function to an alcohol (β -ketoacyl-ACP reductase), dehydration to form an enoyl-ACP (β -hydroxyacyl-ACP dehydrase), and finally reduction of the enoyl-ACP to form the elongated saturated acyl-ACP (enoyl-ACP reductase). β -ketoacyl-ACP synthase I, catalyzes elongation up to palmitoyl-ACP (C16:0), whereas β -ketoacyl-ACP synthase II catalyzes the final elongation to stearoyl-ACP (C18:0). The longest chain fatty acids produced by the

FAS are typically 18 carbons long. Additional biochemical steps in the cell produce specific fatty acid constituents, for example through desaturation and elongation.

5 β -ketoacyl synthases, condensing enzymes, comprise a structurally and functionally related family that play critical roles in the biosynthesis of a variety of natural products, including fatty acids, and the polyketide precursors leading to antibiotics, toxins, and other secondary metabolites. β -ketoacyl synthases catalyze carbon-carbon bond forming reactions by condensing a variety of acyl chain precursors with an elongating carbon source, usually malonyl or methyl malonyl moieties, that are covalently attached through a thioester linkage to an acyl carrier protein. Condensing enzymes can be part of multienzyme complexes, domains of large, multifunctional polypeptide chains as the
10 mammalian fatty acid synthase, or single enzymes as the β -ketoacyl synthases in plants and most bacteria.

Condensing enzymes have been identified with properties subject to exploitation in the areas of plant oil modification, polyketide engineering, and ultimately design anti-cancer and anti-tuberculosis agents. One of the molecular targets of isoniazid, which is widely used in the treatment
15 of tuberculosis, is KAS. Cerulinin, a mycotoxin produced by the fungus *Cephalosporium caerulens*, acts as a potent inhibitor of KAS by covalent modification of the active cysteine thiol. Condensing enzymes from many other pathways and sources have all been shown to be inactivated by this antibiotic with the exception of the synthase from *C. caerulens* and KASIII, the isozyme responsible for the initial condensation of malonyl-ACP with acetyl-CoA in plant and bacterial fatty acid
20 biosynthesis. Inhibition of the KAS domain of fatty acid synthase by cerulinin is selectively cytotoxic to certain cancer cells.

SUMMARY OF THE INVENTION

25 The present invention is directed to β -ketoacyl ACP synthase (KAS), and in particular to engineered KAS polypeptides and polynucleotides encoding engineered KAS proteins having a modified substrate specificity with respect to the native (also referred to herein as wild-type) KAS protein. The engineered polypeptides and polynucleotides of the present invention include
30 those derived from plant and bacterial sources.

In another aspect of the invention polynucleotides encoding engineered polypeptides, particularly, polynucleotides that encode a KAS protein with a modified substrate specificity with respect to the native KAS protein, are provided.

In a further aspect the invention relates to oligonucleotides derived from the engineered KAS proteins and oligonucleotides which include partial or complete engineered KAS encoding sequences.

It is also an aspect of the present invention to provide recombinant DNA constructs which can be used for transcription or transcription and translation (expression) of an engineered KAS protein having an altered substrate specificity with respect to the native KAS protein. In particular, constructs are provided which are capable of transcription or transcription and translation in host cells. Particularly preferred constructs are those capable of transcription or transcription and translation in plant cells.

In another aspect of the present invention, methods are provided for production of engineered KAS proteins having a modified substrate specificity with respect to the native KAS in a host cell or progeny thereof. In particular, host cells are transformed or transfected with a DNA construct which can be used for transcription or transcription and translation of an engineered KAS. The recombinant cells which contain engineered KAS are also part of the present invention.

In a further aspect, the present invention relates to methods of using the engineered polynucleotide and polypeptide sequences of the present invention to modify the fatty acid composition in a host cell, as well as to modify the composition and/or structure of triglyceride molecules, particularly in seed oil of oilseed crops. Plant cells having such a modified triglyceride content are also contemplated herein.

The modified plants, seeds and oils obtained by the expression of the plant engineered KAS proteins are also considered part of the invention.

DESCRIPTION OF THE FIGURES

Figure 1 provides the coordinates of the crystal structure of the *E. coli* KAS protein. The first column provides the Type of atom (N=Nitrogen, O=oxygen, C=Carbon, CA= alpha carbon, CB=beta carbon, CG= gamma carbon, CD= delta carbon, CE= epsilon carbon, NZ=zeta

nitrogen, NH= amino group), the second column provides the amino acid residue type (three letter abbreviation), the third column provides the subunit in which the amino acid is located, the forth column provides the amino acid position in the protein sequence base don the mature unprocessed protein, columns seven through nine provide the x, y and z coordinates, respectively, of the three dimensional location of the respective atom in the crystal structure.

Figure 2 provides the profile of the crystal structure of the *E. coli* KAS-cerulenin complex. The first column provides the Type of atom (N=Nitrogen, O=oxygen, C=Carbon, CA= alpha carbon, CB=beta carbon, CG= gamma carbon, CD= delta carbon, CE= epsilon carbon, NZ= zeta nitrogen, NH= amino group), the second column provides the amino acid residue type (three letter abbreviation), the third column provides the subunit in which the amino acid is located, the forth column provides the amino acid position in the protein sequence base don the mature unprocessed protein, columns seven through nine provide the x, y and z coordinates, respectively, of the three dimensional location of the respective atom in the crystal structure.

Figure 3 provides the effects of KAS II mutations on the fatty acid composition of *E. coli*.

Figure 4 shows that mutations I108F, I108L and A193M all cause significant reduction in the activity of KAS II on 8:0-ACP as compared to 6:0-ACP (38, 31 and 12 fold reductions respectively), without significantly reducing the activity on 6:0-ACP.

Figure 5 shows that the combined mutations at I108 and A193 have the effect of reducing the activity of KAS II on 6:0-ACP substrates.

Figure 6 shows that the combined effect of two or more mutations had a greater effect on the activity with acyl-ACPs 8:0 and longer (14:0) substrates.

Figure 7 shows the complete list of mutations that were generated.

Figure 8 provides the structure of the *Cpu* KAS I homodimer

Figure 9 provides the structure of the *Cpu* KAS IV homodimer

Figure 10 provides the structure of the *Cpu* KAS I/ *Cpu* KAS IV heterodimer.

Figure 11 provides the sequence differences in the hydrophobic pocket of the *E. coli* KASII and *C. pu* KASIV.

Figure 12 provides an amino acid sequence alignment of KAS protein sequences from plant (*Arabidopsis*, *Brassica*, *Cuphea hookeriana* and *pullcherima*, *Hordeum*, *Riccinus*), bacterial (*E. coli*, *streptococcus*, tuberculosis), mammalian (rat, mouse) and others (*C.elegans*).

Figure 13 provides a bar graph representing the results of fatty acid analysis of seeds from transformed *Arabidopsis* lines containing pCGN11058, pCGN11062, pCGN11041, or nontransformed control lines (AT002-44). For each line, bars represent, from left to right, C12:0, C14:0, C16:0, C16:1, C18:0, C18:1 (delta 9), C18:1 (delta 11), C18:2, C18:3, C20:0, C20:1 (delta 11), C20:1 (delta 13), C20:2, C20:3, C22:0, C22:1, C22:2, C22:3, C24:0, and C24:1 fatty acids.

Figure 14 provides the nucleotide sequence of the plastid targeting sequence from *Cuphea hookeriana* KASII-7.

DETAILED DESCRIPTION OF THE INVENTION

In accordance with the subject invention, engineered nucleotide sequences are provided which are capable of coding sequences of amino acids, such as, a protein, polypeptide or peptide. The engineered nucleotide sequences encode β -ketoacyl-ACP synthase (KAS) proteins with a modified substrate specificity compared to the native KAS protein (also referred to herein as the wild-type KAS protein) under enzyme reaction conditions. Such sequences are referred to herein as engineered β -ketoacyl-ACP synthase (also referred to as engineered KAS) proteins. The engineered nucleic acid sequences find use in the preparation of constructs to direct their expression in a host cell. Furthermore, the engineered nucleic acid sequences find use in the preparation of plant expression constructs to alter the fatty acid composition of a plant cell. By "enzyme reactive conditions" is meant that any necessary conditions are available in an environment (for example, such factors as temperature, pH, lack of inhibiting substances) which will permit the enzyme to function.

An engineered β -ketoacyl-ACP synthase nucleic acid sequence of this invention includes any nucleic acid sequence coding a β -ketoacyl-ACP synthase having altered substrate specificity relative to the native KAS in a host cell, including but not limited to, *in vivo*, or in a cell-like environment, for example, *in vitro*. By altered, or modified, substrate specificity is meant an alteration in the acyl-ACP substrates elongated by the KAS enzyme or an alteration in the elongator molecule used by the KAS to elongate the acyl-ACP relative to the native or unaltered KAS protein. An alteration in the acyl-ACP substrate elongated by the KAS enzymes includes,

but is not limited to, elongation of an acyl-ACP substrate not elongated by the wild-type KAS, the inability to elongate an acyl-ACP substrate elongated by the wild-type KAS, and a preference for elongating acyl-ACP substrates not normally preferred by the wild-type KAS. An alteration in the elongator molecule used by the engineered KAS for the elongation of the acyl-ACP substrate includes, but is not limited to, methyl-malonyl ACP for the production of branched chain fatty acids.

A first aspect of the present invention relates to engineered β -ketoacyl-ACP synthase polypeptides. In particular, engineered KAS II polypeptides are provided. Preferred peptides include those found in the hydrophobic fatty acid/cerulenin binding pocket of the KAS protein. Such polypeptides include the engineered polypeptides set forth in the Sequence Listing, as well as polypeptides and fragments thereof, particularly those polypeptides which exhibit a modified substrate specificity with respect to the wild-type KAS polypeptide. Particularly preferred polypeptides include those having engineered amino acid residues 105 to 120, 130-140, 190-200 and 340-400. Most preferred polypeptides include those having engineered amino acid residues I108A, I108F, I108G, I108L, L111A, I114A, F133A, V134A, V134G, I138A, I138G, A162G, A193G, A193I, A193M, L197A, F202L, F202I, F202G, L342A, and L342G. Amino acid positions, as used herein, refer to the amino acid residue position in the active or processed protein.

Engineered β -ketoacyl-ACP synthases can be prepared by random (via chemical mutagenesis or DNA shuffling) or specific mutagenesis of a β -ketoacyl-ACP synthase encoding sequence to provide for one or more amino acid substitutions in the translated amino acid sequence. Alternatively, an engineered β -ketoacyl-ACP synthase can be prepared by domain swapping between related β -ketoacyl-ACP synthases, wherein extensive regions of the native β -ketoacyl-ACP synthase encoding sequence are replaced with the corresponding region from a different β -ketoacyl-ACP synthase.

Altered substrate specificities of an engineered β -ketoacyl-ACP synthase can be reflected by the elongation of an acyl-ACP substrates of particular chain length fatty acyl-ACP groups which are not elongated by the native β -ketoacyl-ACP synthase enzyme. In addition, altered substrate specificities can be reflected by the inability to elongate an acyl-ACP substrate of

particular chain length fatty acyl-ACP groups which are not normally preferred by the native β -ketoacyl-ACP synthase enzyme. The newly recognized acyl-ACP substrate can differ from native substrates of the enzyme in various ways, such as by having a shorter or longer carbon chain length (usually reflected by the addition or deletion of one or more 2-carbon units), as well as by degrees of unsaturation.

Another aspect of the present invention relates to engineered β -ketoacyl-ACP synthase polynucleotides. In particular, engineered β -ketoacyl-ACP synthase II polynucleotides are provided. The polynucleotide sequences of the present invention include engineered polynucleotides that encode the polypeptides of the invention having a deduced amino acid sequence selected from the group of sequences set forth in the Sequence Listing.

The invention provides a polynucleotide sequence identical over its entire length to each coding sequence as set forth in the Sequence Listing. The invention also provides the coding sequence for the mature polypeptide or a fragment thereof, as well as the coding sequence for the mature engineered polypeptide or a fragment thereof in a reading frame with other coding sequences, such as those encoding a leader or secretory sequence, a pre-, pro-, or prepro- protein sequence. The polynucleotide can also include non-coding sequences, including for example, but not limited to, non-coding 5' and 3' sequences, such as the transcribed, untranslated sequences, termination signals, ribosome binding sites, sequences that stabilize mRNA, introns, polyadenylation signals, and additional coding sequence that encodes additional amino acids. For example, a marker sequence can be included to facilitate the purification of the fused polypeptide. Polynucleotides of the present invention also include polynucleotides comprising a structural gene and the naturally associated sequences that control gene expression.

As described herein, analysis of the KAS II/cerulinin crystal structure complex is performed using modeling software to produce a profile of the complex, as well as the KAS II protein alone. Based on comparisons of the two profiles, amino acid residues are identified, which when mutagenized, alter the fatty acyl substrate specificities. As demonstrated herein, engineering of the nucleic acid sequence to modify the amino acid sequence in particular regions of the KAS protein effectively modify the substrate specificity of the engineered KAS. Particular ranges for the engineering of the protein include amino acid residues 105 to 120, 130-140, 190-200 and 340-345. Particularly, engineering of residues 108, 111, 114, 133, 193 and 197 can alter

the length of the fatty acids synthesized by the engineered KAS II protein. More particularly, engineering of residues 108, 111, 114, 133, 193 and 197 with variously sized hydrophobic residues will alter the length of the fatty acids synthesized by the engineered KAS II protein. Furthermore, engineering the amino acid residue at position 400 can also have an effect on the substrate specificity.

As demonstrated more fully in the following examples, the acyl-ACP substrate specificity of b-ketoacyl-ACP synthases may be modified by various amino acid changes to the protein sequence, such as amino acid substitutions, insertions or deletions in the mature protein portion of the b-ketoacyl-ACP synthases. Modified substrate specificity can be detected by expression of the engineered b-ketoacyl-ACP synthase s in *E. coli* and assaying to detect enzyme activity or by using purified protein in *in vitro* assays.

Modified substrate specificity can be indicted by a shift in acyl-ACP substrate preference such that the engineered b-ketoacyl-ACP synthase is newly capable of utilizing a substrate not recognized by the native b-ketoacyl-ACP synthase . The newly recognized substrate can vary from substrates of the native enzyme by carbon chain length and/or degree of saturation of the fatty acyl portion of the substrate. Additionally, modified substrate specificity can be reflected by a shift in the relative b-ketoacyl-ACP synthase activity on two or more substrates of the native b-ketoacyl-ACP synthase such that an engineered b-ketoacyl-ACP synthase exhibits a different order of preference for the acyl-ACP substrates.

Furthermore, provided herein are KAS proteins with an altered elongator molecule preference. For example, by widening the hydrophobic fatty acid binding different elongator molecules, other than Malonyl-ACP, can be utilized by the KAS protein. For example Methyl-malonyl-ACP can be utilized by the engineered KAS resulting in the synthesis of branched chained fatty acid. The mutations that lengthen the pocket may to some degree also widen it, in addition mutations A193G, I108G, L342A or G, V134A or G, F202L, I or G may well cause widening of the pocket sufficiently to allow Methyl-malonyl-ACP to be accepted as an elongator.

As described in more detail herein, alterations in the nucleic acid sequence of the *E. coli* KAS II, particularly, I108F, I108L, A193I, A193M, as well as combinations thereof, are prepared for the production of shorter chain length fatty acids. Furthermore, alterations of I108A, L111A,

I114A, F133A, L197A, and combinations thereof, are prepared for increasing the length of fatty acids produced by the host cell.

Thus, as the result of modifications to the substrate specificity of b-ketoacyl-ACP synthases, it can be seen that the relative amounts of the fatty acids produced in a cell where various substrates are available for hydrolysis may be altered. Furthermore, molecules which are formed from available free fatty acids, such as plant seed triglycerides, may also be altered as a result of expression of engineered b-ketoacyl-ACP synthase s having altered substrate specificities.

It is anticipated that the ranges of mutations provided herein can also be engineered in plant KAS proteins as well as to other polyketide synthases. Such plant KAS proteins are known in the art, and are described for example in PCT Publication WO 98/46776, and in U.S. Patent Number 5,475,099, the entireties of which are incorporated herein by reference.

Plant Constructs and Methods of Use

Of particular interest is the use of the nucleotide sequences, or polynucleotides, in recombinant DNA constructs to direct the transcription or transcription and translation (expression) of the engineered KAS sequences of the present invention in a host plant cell. The expression constructs generally comprise a promoter functional in a host plant cell operably linked to a nucleic acid sequence encoding a engineered KAS of the present invention and a transcriptional termination region functional in a host plant cell.

Those skilled in the art will recognize that there are a number of promoters which are functional in plant cells, and have been described in the literature. Chloroplast and plastid specific promoters, chloroplast or plastid functional promoters, and chloroplast or plastid operable promoters are also envisioned.

One set of promoters are constitutive promoters such as the CaMV35S or FMV35S promoters that yield high levels of expression in most plant organs. Enhanced or duplicated versions of the CaMV35S and FMV35S promoters are useful in the practice of this invention (Odell, *et al.* (1985) *Nature* 313:810-812; Rogers, U.S. Patent Number 5,378, 619). In addition, it may also be preferred to bring about expression of the engineered KAS in specific tissues of the

plant, such as leaf, stem, root, tuber, seed, fruit, etc., and the promoter chosen should have the desired tissue and developmental specificity.

Of particular interest is the expression of the nucleic acid sequences of the present invention from transcription initiation regions which are preferentially expressed in a plant seed tissue. Examples of such seed preferential transcription initiation sequences include those sequences derived from sequences encoding plant storage protein genes or from genes involved in fatty acid biosynthesis in oilseeds. Examples of such promoters include the 5' regulatory regions from such genes as napin (Kridl *et al.*, *Seed Sci. Res.* 1:209:219 (1991)), phaseolin, zein, soybean trypsin inhibitor, ACP, stearyl-ACP desaturase, soybean α' subunit of β -conglycinin (soy 7s, (Chen *et al.*, *Proc. Natl. Acad. Sci.*, 83:8560-8564 (1986))) and oleosin.

It may be advantageous to direct the localization of proteins to a particular subcellular compartment, for example, to the mitochondrion, endoplasmic reticulum, vacuoles, chloroplast or other plastidic compartment. For example, where the genes of interest of the present invention will be targeted to plastids, such as chloroplasts, for expression, the constructs will also employ the use of sequences to direct the gene to the plastid. Such sequences are referred to herein as chloroplast transit peptides (CTP) or plastid transit peptides (PTP). In this manner, where the protein of interest is not directly inserted into the plastid, the expression construct will additionally contain a gene encoding a transit peptide to direct the protein of interest to the plastid. The chloroplast transit peptides may be derived from the gene of interest, or may be derived from a heterologous sequence having a CTP. Such transit peptides are known in the art. See, for example, Von Heijne *et al.* (1991) *Plant Mol. Biol. Rep.* 9:104-126; Clark *et al.* (1989) *J. Biol. Chem.* 264:17544-17550; della-Cioppa *et al.* (1987) *Plant Physiol.* 84:965-968; Romer *et al.* (1993) *Biochem. Biophys. Res Commun.* 196:1414-1421; and, Shah *et al.* (1986) *Science* 233:478-481. Additional transit peptides for the translocation of the engineered KAS protein to the endoplasmic reticulum (ER), or vacuole may also find use in the constructs of the present invention.

Depending upon the intended use, additional constructs can be employed containing the nucleic acid sequence which provides for the suppression of the host cell's endogenous KAS protein. Where antisense inhibition of a host cells native KAS protein is desired, the entire wild-type KAS sequence is not required.

The skilled artisan will recognize that there are various methods for the inhibition of expression of endogenous sequences in a host cell. Such methods include, but are not limited to antisense suppression (Smith, *et al.* (1988) *Nature* 334:724-726), co-suppression (Napoli, *et al.* (1989) *Plant Cell* 2:279-289), ribozymes (PCT Publication WO 97/10328), and combinations of sense and antisense Waterhouse, *et al.* (1998) *Proc. Natl. Acad. Sci. USA* 95:13959-13964. Methods for the suppression of endogenous sequences in a host cell typically employ the transcription or transcription and translation of at least a portion of the sequence to be suppressed. Such sequences may be homologous to coding as well as non-coding regions of the endogenous sequence.

Regulatory transcript termination regions may be provided in plant expression constructs of this invention as well. Transcript termination regions may be provided by the DNA sequence encoding the wild-type KAS or a convenient transcription termination region derived from a different gene source, for example, the transcript termination region which is naturally associated with the transcript initiation region. The skilled artisan will recognize that any convenient transcript termination region which is capable of terminating transcription in a plant cell may be employed in the constructs of the present invention.

Alternatively, constructs may be prepared to direct the expression of the engineered KAS sequences directly from the host plant cell plastid. Such constructs and methods are known in the art and are generally described, for example, in Svab, *et al.* (1990) *Proc. Natl. Acad. Sci. USA* 87:8526-8530 and Svab and Maliga (1993) *Proc. Natl. Acad. Sci. USA* 90:913-917 and in U.S. Patent Number 5,693,507.

A plant cell, tissue, organ, or plant into which the recombinant DNA constructs containing the expression constructs have been introduced is considered transformed, transfected, or transgenic. A transgenic or transformed cell or plant also includes progeny of the cell or plant and progeny produced from a breeding program employing such a transgenic plant as a parent in a cross and exhibiting an altered phenotype resulting from the presence of a engineered KAS nucleic acid sequence.

Plant expression or transcription constructs having an engineered KAS as the DNA sequence of interest for increased or decreased expression thereof may be employed with a wide variety of plant life, particularly, plant life involved in the production of vegetable oils for edible

and industrial uses. Most especially preferred are temperate oilseed crops. Plants of interest include, but are not limited to, rapeseed (Canola and High Erucic Acid varieties), sunflower, safflower, cotton, soybean, peanut, coconut and oil palms, and corn. Depending on the method for introducing the recombinant constructs into the host cell, other DNA sequences may be required. Importantly, this invention is applicable to dicotyledons and monocotyledons species alike and will be readily applicable to new and/or improved transformation and regulation techniques.

Of particular interest, is the use of engineered KAS constructs in plants which have been genetically engineered to produce a particular fatty acid in the plant seed oil, where TAG in the seeds of nonengineered plants of the engineered species, do not naturally contain that particular fatty acid.

The engineered KAS constructs of the present invention can also be used to provide a means for the production of plants having resistance to plant pathogens. Engineered KAS constructs providing for an increased production of particular fatty acids involved in the biosynthesis of pathogen response signals or inhibitors. For example, engineered KAS constructs providing for the increased production of C:8 fatty acids allows for the production of transgenic plants having an increased tolerance to fungal pathogens.

It is contemplated that the gene sequences may be synthesized, either completely or in part, especially where it is desirable to provide plant-preferred sequences. Thus, all or a portion of the desired structural gene (that portion of the gene which encodes the engineered protein) may be synthesized using codons preferred by a selected host. Host-preferred codons may be determined, for example, from the codons used most frequently in the proteins expressed in a desired host species.

Once the desired engineered KAS nucleic acid sequence is obtained, it may be manipulated in a variety of ways. Where the sequence involves non-coding flanking regions, the flanking regions may be subjected to resection, mutagenesis, etc. Thus, transitions, transversions, deletions, and insertions may be performed on the naturally occurring sequence. In addition, all or part of the sequence may be synthesized. In the structural gene, one or more codons may be modified to provide for a modified amino acid sequence, or one or more codon mutations may be introduced to provide for a convenient restriction site or other purpose

involved with construction or expression. The structural gene may be further modified by employing synthetic adapters, linkers to introduce one or more convenient restriction sites, or the like.

The nucleic acid or amino acid sequences encoding an engineered KAS of this invention may be combined with other non-native, or "heterologous", sequences in a variety of ways. By "heterologous" sequences is meant any sequence which is not naturally found joined to the engineered KAS, including, for example, combinations of nucleic acid sequences from the same plant which are not naturally found joined together.

The DNA sequence encoding an engineered KAS of this invention may be employed in conjunction with all or part of the gene sequences normally associated with the wild-type KAS. In its component parts, a DNA sequence encoding engineered KAS is combined in a DNA construct having, in the 5' to 3' direction of transcription, a transcription initiation control region capable of promoting transcription and translation in a host cell, the DNA sequence encoding engineered KAS and a transcription and translation termination region.

Potential host cells include both prokaryotic and eukaryotic cells. A host cell may be unicellular or found in a multicellular differentiated or undifferentiated organism depending upon the intended use. Cells of this invention may be distinguished by having an engineered KAS foreign to the wild-type cell present therein, for example, by having a recombinant nucleic acid construct encoding an engineered KAS therein.

The methods used for the transformation of the host plant cell are not critical to the present invention. The transformation of the plant is preferably permanent, i.e. by integration of the introduced expression constructs into the host plant genome, so that the introduced constructs are passed onto successive plant generations. The skilled artisan will recognize that a wide variety of transformation techniques exist in the art, and new techniques are continually becoming available. Any technique that is suitable for the target host plant can be employed within the scope of the present invention. For example, the constructs can be introduced in a variety of forms including, but not limited to as a strand of DNA, in a plasmid, or in an artificial chromosome. The introduction of the constructs into the target plant cells can be accomplished by a variety of techniques, including, but not limited to calcium-phosphate-DNA co-precipitation, electroporation, microinjection, *Agrobacterium* infection, liposomes or

microprojectile transformation. The skilled artisan can refer to the literature for details and select suitable techniques for use in the methods of the present invention.

Normally, included with the DNA construct will be a structural gene having the necessary regulatory regions for expression in a host and providing for selection of transformant cells. The gene may provide for resistance to a cytotoxic agent, e.g. antibiotic, heavy metal, toxin, etc., complementation providing prototrophy to an auxotrophic host, viral immunity or the like. Depending upon the number of different host species the expression construct or components thereof are introduced, one or more markers may be employed, where different conditions for selection are used for the different hosts.

Where *Agrobacterium* is used for plant cell transformation, a vector may be used which may be introduced into the *Agrobacterium* host for homologous recombination with T-DNA or the Ti- or Ri-plasmid present in the *Agrobacterium* host. The Ti- or Ri-plasmid containing the T-DNA for recombination may be armed (capable of causing gall formation) or disarmed (incapable of causing gall formation), the latter being permissible, so long as the *vir* genes are present in the transformed *Agrobacterium* host. The armed plasmid can give a mixture of normal plant cells and gall.

In some instances where *Agrobacterium* is used as the vehicle for transforming host plant cells, the expression or transcription construct bordered by the T-DNA border region(s) will be inserted into a broad host range vector capable of replication in *E. coli* and *Agrobacterium*, there being broad host range vectors described in the literature. Commonly used is pRK2 or derivatives thereof. See, for example, Ditta, *et al.*, (*Proc. Nat. Acad. Sci., U.S.A.* (1980) 77:7347-7351) and EPA 0 120 515, which are incorporated herein by reference. Alternatively, one may insert the sequences to be expressed in plant cells into a vector containing separate replication sequences, one of which stabilizes the vector in *E. coli*, and the other in *Agrobacterium*. See, for example, McBride and Summerfelt (*Plant Mol. Biol.* (1990) 14:269-276), wherein the pRiHRI (Jouanin, *et al.*, *Mol. Gen. Genet.* (1985) 201:370-374) origin of replication is utilized and provides for added stability of the plant expression vectors in host *Agrobacterium* cells.

Included with the expression construct and the T-DNA will be one or more markers, which allow for selection of transformed *Agrobacterium* and transformed plant cells. A number

of markers have been developed for use with plant cells, such as resistance to chloramphenicol, kanamycin, the aminoglycoside G418, hygromycin, or the like. The particular marker employed is not essential to this invention, one or another marker being preferred depending on the particular host and the manner of construction.

5 For transformation of plant cells using *Agrobacterium*, explants may be combined and incubated with the transformed *Agrobacterium* for sufficient time for transformation, the bacteria killed, and the plant cells cultured in an appropriate selective medium. Once callus forms, shoot formation can be encouraged by employing the appropriate plant hormones in accordance with known methods and the shoots transferred to rooting medium for regeneration of plants. The
10 plants may then be grown to seed and the seed used to establish repetitive generations and for isolation of vegetable oils.

There are several possible ways to obtain the plant cells of this invention which contain multiple expression constructs. Any means for producing a plant comprising a construct having a DNA sequence encoding the engineered KAS of the present invention, and at least one other
15 construct having another DNA sequence encoding an enzyme are encompassed by the present invention. For example, the expression construct can be used to transform a plant at the same time as the second construct either by inclusion of both expression constructs in a single transformation vector or by using separate vectors, each of which express desired genes. The second construct can be introduced into a plant which has already been transformed with the
20 engineered KAS expression construct, or alternatively, transformed plants, one expressing the engineered KAS construct and one expressing the second construct, can be crossed to bring the constructs together in the same plant.

Other Constructs and Methods of Use

25 The invention also relates to vectors that include a polynucleotide or polynucleotides of the invention, host cells that are genetically engineered with vectors of the invention and the production of polypeptides of the invention by recombinant techniques. Cell free translation systems can be employed to produce such protein using RNAs derived from the DNA constructs of the invention.

For recombinant production, host cells can be genetically engineered to incorporate expression systems or portions thereof or polynucleotides of the present invention. Introduction of a polynucleotide into a host cell can be effected by methods described in many standard laboratory manuals, such as Davis et al., *Basic Methods in Molecular Biology*, (1986) and
5 Sambrook et al, *Molecular Cloning: A Laboratory Manual*, 2nd Edition, Cold Spring Harbor Laboratory Press, Cold Spring Harbor NY (1989). Such methods include, but are not limited to, calcium phosphate transfection, DEAE dextran mediated transfection, transvection, microinjection, cationic lipid-mediated transfection, electroporation, transduction, scrape loading ballistic introduction and infection.

10 Representative examples of appropriate hosts include bacterial cells, such as streptococci, staphylococci, enterococci, *E. coli*, streptomyces, and *Bacillus subtilis* cells; fungal cells, such as yeast cells and *Aspergillus* cells; insect cells, such as *Drosophila* S2 and *Spodoptera* Sf9 cells; animal cells such as CHO, COS, HeLa, C127, 3T3, BHK, 293 and Bowes melanoma cells; and plant cells as described above.

15 A variety of expression systems can be used to produce the polypeptides of the invention. Such vectors include, but are not limited to, chromosomal, episomal, and virus derived vectors, for example vectors from bacterial plasmids, bacteriophage, transposons, yeast episomes, insertion elements, yeast chromosomal elements, viruses such as baculoviruses, papova viruses, such as SB40, vaccinia viruses, adenoviruses, fowl pox viruses, pseudorabies viruses and
20 retroviruses, and vectors derived from combinations of such viruses, such as those derived from plasmid and bacteriophage genetic elements, such as cosmids and phagemids. The expression system constructs may contain control regions that regulate as well as engender expression. Generally, any system or vector which is suitable to maintain, propagate or express polynucleotides and/or to express a polypeptide in a host can be used for expression. The
25 appropriate DNA sequence can be inserted into the chosen expression by any of a variety of well-known and routine techniques, such as, for example, those set forth in Sambrook et al, *Molecular Cloning, A Laboratory Manual*, (*supra*).

30 Appropriate secretion signals, either homologous or heterologous, can be incorporated into the expressed polypeptide to allow the secretion of the protein into the lumen of the endoplasmic reticulum, the periplasmic space or the extracellular environment.

The polypeptides of the present invention can be recovered and purified from recombinant cell cultures by any of a number of well known methods, including, but not limited to, ammonium sulfate or ethanol precipitation, acid extraction, anion or cation exchange chromatography, phosphocellulose chromatography, hydrophobic interaction chromatography, affinity chromatography, hydroxylapatite chromatography, and lectin chromatography. It is most preferable to use high performance liquid chromatography (HPLC) for purification. Any of the well known techniques for protein refolding can be used to regenerate an active confirmation if the polypeptide is denatured during isolation and/or purification.

The engineered KAS polynucleotides and polypeptides of the present invention find use in a variety of applications.

The engineered KAS polynucleotides and polypeptides as well as the constructs containing such engineered KAS polynucleotides and polypeptides find use in the alteration of fatty acid composition. Furthermore, the engineered KAS polynucleotides and polypeptides of the present invention find use in the production of particular fatty acid components. For example, an engineered KAS having a preference for elongating 6, 8, 10, and 12 carbon acyl-ACP substrates can be used in the production of medium chain fatty acids. Such engineered KAS polynucleotides and polypeptides can also be used with additional sequences for the production of medium chain fatty acids, including, but not limited to, medium chain specific thioesterases (see for example USPN 5,512,482).

The present invention further provides methods for the engineering of polyketides and for the identification of molecules useful in cancer therapy, immunosuppressants, anti-parasite, and antibiotic production.

Thus, the present invention permits the use of molecular design techniques to design, select and synthesize chemical entities and compounds, including inhibitory compounds, capable of binding to the active site or substrate binding site of KAS, in whole or in part.

A first approach enabled by this invention, is to use the structure coordinates of KAS to design compounds that bind to the enzyme and alter the physical properties of the compounds in different ways, e.g., solubility. For example, this invention enables the design of compounds that act as competitive inhibitors of the KAS enzyme by binding to, all or a portion of, the active site of KAS. This invention also enables the design of compounds that act as uncompetitive

inhibitors of the KAS enzyme. These inhibitors may bind to, all or a portion of, the substrate binding site of KAS already bound to its substrate and may be more potent and less non-specific than known competitive inhibitors that compete only for the KAS active site. Similarly, non-competitive inhibitors that bind to and inhibit KAS whether or not it is bound to another chemical entity may be designed using the structure coordinates of KAS of this invention. Additionally, reversible and irreversible inhibitors can also be designed.

A second design approach is to probe KAS with molecules composed of a variety of different chemical entities to determine optimal sites for interaction between candidate ICE inhibitors and the enzyme. For example, high resolution X-ray diffraction data collected from crystals saturated with solvent allows the determination of where each type of solvent molecule sticks. Small molecules that bind tightly to those sites can then be designed and synthesized and tested for their KAS inhibitor activity. Travis, J., *Science*, 262, p. 1374 (1993).

This invention also enables the development of compounds that can isomerize to short-lived reaction intermediates in the chemical reaction of a substrate or other compound that binds to KAS, with KAS. Thus, the time-dependent analysis of structural changes in KAS during its interaction with other molecules is enabled. The reaction intermediates of KAS can also be deduced from the reaction product in co-complex with KAS. Such information is useful to design improved analogues of known KAS inhibitors or to design novel classes of inhibitors based on the reaction intermediates of the KAS enzyme and KAS-inhibitor co-complex. This provides a novel route for designing KAS inhibitors with both high specificity and stability.

Another approach made possible and enabled by this invention, is to screen computationally small molecule data bases for chemical entities or compounds that can bind in whole, or in part, to the KAS enzyme. In this screening, the quality of fit of such entities or compounds to the binding site may be judged either by shape complementarity or by estimated interaction energy. Meng, E. C. *et al.*, *J. Comp. Chem.*, 13, pp. 505-524 (1992).

The invention now being generally described, it will be more readily understood by reference to the following examples which are included for purposes of illustration only and are not intended to limit the present invention.

EXAMPLES

Example 1: Determination of the KAS II-Ceruleinin Complex Structure

5 The KASII-ceruleinin complex was prepared as described previously (Edwards, *et al.* (1997) *FEBS Lett.* 402:62-66). Crystals of the complex were grown by the hanging drop method. Droplets consisting of equal amounts of protein solution (6 mg ml⁻¹, 21 protein, 0.3 M NaCl, 25 mM Tris, pH 8.0, 5 mM Imidazole, and 10% v/v glycerol) and reservoir solution were equilibrated against 26% w/v polyethylene glycol 8000 and 0.1% v/v 2-mercaptoethanol in water.

10 Data from two crystals were collected at 298 K at the synchrotron in MAX-lab, beamline I711, in Lund. The data was processed with DENZO (Otwinowski (1993) *Proceedings of the Collaborative Computing Project 4 Study Weekend: Data Collection and Processing* (Sawyer, L., Isaacs, N., and Bailey, S.S., eds.) pp 56-62, SERC Daresbury Laboratory, Warrington) and programs from the Collaborative Computing Project 4 Suite (Collaborative Computing

15 Project 4 (1994) *Acta Crystallogr. Sect. D Biol. Crystallogr.* 50:760-763) and the two data sets were scaled together in SCALA (Evans, (1993) *Proceedings of the Collaborative Computing Project 4 Study Weekend: Data Collection and Processing* (Sawyer, L., Isaacs, N., and Bailey, S.S., eds.) pp 56-62, SERC Daresbury Laboratory, Warrington). The crystals are very radiation-sensitive, but cannot be frozen in a cryostream. Due to non-isomorphism, data of only two

20 crystals could be merged. The crystals of the complex have space group P3₂1 with similar cell dimensions as the native enzyme. The coordinates of the native enzyme (Huang, *et al.* (1998) *EMBO J.* 17:1183-1191) were used to calculate initial electron density maps with SIGMAA (Read (1986) *Acta Crystallogr.* 42:140-149). All data were used in the refinement; no sigma cutoff was applied. After an initial cycle of positional refinement, the model was rebuilt and a

25 model of ceruleinin was included. Further cycles of refinement of the complex were carried out using the program REFMAC (Murshudov, *et al.* (1997) *Acta Crystallogr. Sect. D Biol. Crystallogr.* 53:240-253) including a bulk solvent correction, interspersed with inspection and correction of the model using O (Jones, *et al.* (1991) *Acta Crystallogr. Sect. A* 47:100-119), OOPS (Kleywegt, *et al.* (1996) *Acta Crystallogr. Sect. D Biol. Crystallogr.* 52:829-832), and

PROCHECK (Laskowski, *et al.* (1993) *J. Appl. Crystallogr.* 26:282-291). Structure comparisons were performed using O (Jones, *et al.* (1991) *supra*) with default parameters.

The complex of KASII from *E. coli* with cerulenin crystallized in space group P3₁21 isomorphously with the native enzyme (Huang, *et al.* (1998) *supra*), and the crystal structure was determined to 2.65-Å resolution by difference Fourier methods. The final protein model after refinement (R -factor 5 0.213 and R_{free} 5 0.270 with good stereochemistry) contains 411 out of the 412 residues of the subunit; no electron density for the N-terminal residue was found. The overall real-space correlation coefficient (Jones, *et al.* (1991) *supra*) is 0.92, and there is well defined electron density for the polypeptide chain except for some side chains on the molecular surface.

The inhibitor molecule is well defined by the electron density. However, there is weaker than average electron density for the amide group and no electron density for the last carbon atom of the hydrocarbon tail, indicating considerable flexibility for the terminal methyl group.

The overall structure of the KAS dimer is unchanged upon binding of cerulenin; the root mean square deviations for the 411 C α atoms of the subunit is 0.23 Å between the two structures.

These differences are mainly localized in the active site, in particular in the loop comprising residues 398–401. The main differences in structure between the native enzyme and the cerulenin complex are in the conformation of the side chains of Phe-400 (which was anticipated already from the native structure) and of Ile-108, which have completely new rotamer conformations, and in the positions of the side chains of Cys-163, His-340, and Leu-342, which also have moved substantially. These conformational changes provide access for cerulenin to the active site cysteine and open a hydrophobic pocket for the hydrophobic tail of the inhibitor. From the initial $F_o - F_c$ electron density map these structural changes could be readily seen as well as the binding site for the inhibitor). Cerulenin is bound covalently through its C2 carbon atom to the Cys-163 S γ atom. Its hydrocarbon tail fits in a hydrophobic pocket formed at the dimer interface. The structure of the adduct of cerulenin and cysteine, isolated by tryptic digestion of the cerulenin-fatty acid synthase complex, has been determined by NMR and mass spectroscopy (Funabashi, *et al.* (1989) *J. Biochem.(Tokyo)* 105:751-755). This study revealed that the inhibitor reacts at its C2-epoxide carbon with the SH group of cysteine and that cerulenin formed a hydroxylactam ring. The electron density observed in the KASII-cerulenin complex is not consistent with this structure. It was not possible to model bound cerulenin in the closed ring form but the open form

of the inhibitor could readily be fitted to the electron density map. The hydroxylactam ring, which is formed preferably in protic solvents (Funabashi, *et al.* (1989) *supra*), is not present in the hydrophobic environment of the protein.

In the KASII-cerulenin complex, the inhibitor amide carbonyl oxygen is within hydrogen bond distance to the Ne atoms of the side chains of His-340 and His-303, while the amide NH₂ group does not make any close interactions. It is, however, not possible from the structure to exclude the opposite conformation and interactions for the amide group. The hydroxyl group at C3 forms a hydrogen bond to the main chain NH of Phe-400. The carbonyl oxygen at C4 does not form any polar interactions, in fact, it is located in a very hydrophobic pocket formed by side chains Phe-400, Phe-202, and Val-134 from the other subunit in the dimer. The binding site for the hydrophobic part of the inhibitor is also lined with hydrophobic residues: Ala-162, Gly-107, Leu-342, Phe-202, Leu-111, Ile-108, Ala-193, Gly-198; and from the second subunit in the dimer, Ile-138, Val-134, and Phe-133. The two double bonds with *trans* configuration give the hydrophobic tail a shape that fits to the hydrophobic groove once residue Ile-108 has changed rotamer. In comparison, binding of tetrahydrocerulenin would cost entropy, and as expected it shows more than 2 orders of magnitude less inhibitory activity (D'Agnolo, *et al.* (1973) *Biochim. Biophys. Acta* 326:155-156). The influence of the length of the hydrocarbon chain, maintaining the double bond positions, has been studied using fatty acid synthase from *Saccharomyces cerevisiae* (Morisaki, *et al.* (1993) *J. Biol. Chem.* 211:111-115). Cerulenin (12 carbons) had the highest inhibitory activity, with slightly decreasing binding strength upon increase in chain length. However, when increasing the length from 16 to 18 carbon atoms, the inhibition decreased by 2 orders of magnitude. The size of the hydrophobic pocket in KASII, which binds the hydrocarbon tail of cerulenin, suggests that there is space for a longer hydrophobic tail only if the side chains of Leu-111 and of Phe-133 in the second subunit change their conformation. Thus, possible differences in the sensitivity of condensing enzymes toward cerulenin might be controlled by the size of this cavity.

The structure of the cerulenin complex can be considered to mimic the intermediate formed upon reaction of KAS with the acyl-ACP. In such a complex the hydrophobic cavity would harbor the hydrocarbon tail of the acyl intermediate. The acyl hydrophobic tails will not be restricted by two double bonds (as in the case of cerulenin), and this will allow longer acyl chains

to be buried in this pocket. Inspection of the active site cavity suggests that it would not be possible to harbor a linear acyl chain longer than 14 carbon atoms without structural changes. Such conformational changes must occur since KASII is able to elongate 16:1 to 18:1 (Garwin, *et al.* (1980) *J. Biol. Chem.* 255:3263-3265).

Coordinates for the KAS II crystal structure as well as the KAS-cerulenin complex were produced and are presented in Figures 1 and 2 respectively.

Example 2: Engineering KAS II Proteins

The structure of the *E.coli* KAS II-cerulenin complex was analyzed using the Swiss Pdb Viewer (SPV) modeling program, and by stereo viewing of printouts of the structure in different orientations. Using SPV each of the hydrophobic residues surrounding the bound cerulenin residue were changed to all the possible larger hydrophobic residues, and each of the rotamers for the mutant amino acids were examined for steric clashes (SPV rotamer score) with adjacent amino acids and the bound cerulenin molecule. The identified amino acids were targeted for mutagenesis for decreasing the fatty acid chain length specificity of the KAS II protein. The candidate chain length shortening mutations chosen were those that made the least steric clashes with neighboring amino acids while having the most clashes with the end 1 to 6 carbons of cerulenin.

The structure of the *E.coli* KAS II / cerulenin complex was studied as described above and the hydrophobic amino acid residues near the end of the cerulenin binding "pocket" were identified. These amino acids were identified for mutagenesis for the increase in fatty acid chain length recognition. The large hydrophobic residues positioned beyond the end of the cerulenin potentially preventing longer fatty acids from occupying this pocket were chosen for mutagenesis to smaller (alanine) residues.

PCR site-directed mutagenesis was performed using the Quick-Change™ site-directed mutagenesis kit (Stratagene) following the manufacturers protocol. For the preparation of the specific mutations listed in Table 1, the following oligonucleotide primers were used in the reactions.

Table 1

	I108F Sense	5'-GTGCCGCAATTGGATCCGGGTTTGGCGGCCTCGGAC	(SEQ ID NO:1)
	Antisense	5'-GTCCGAGGCCGCCAAACCCGGATCCAATTGCGGCAC	(SEQ ID NO:2)
5	I108L Sense	5'-GTGCCGCAATTGGCTCCGGGCTTGGAGGCCTCGGACTGATCG	(SEQ ID NO:3)
	Antisense	5'-CGATCAGTCCGAGGCCTCCAAGCCCGAGCCAATTGCGGCAC	(SEQ ID NO:4)
	A193I Sense	5'-GCAGGTGGCGCCGAGAAAATCAGTACGCCGCTGGGC	(SEQ ID NO:5)
	Antisense	5'-GCCCAGCGGCGTACTGATTTTCTCGGCGCCACCTGC	(SEQ ID NO:6)
10	A193M Sense	5'-GGTGGCGCAGAGAAAATGAGTACTCCGCTGGGCGTTG	(SEQ ID NO:7)
	Antisense	5'-CAACGCCAGCGGAGTACTCATTTTCTCTGCGCCACC	(SEQ ID NO:8)
15	I108A, L111A, I114A Sense	5'-GCAATTGGCTCCGGGGCTGGCGGCGCCGGACTGGCCGAAG AAAACCACAC	(SEQ ID NO:9)
	Antisense	5'-GTGTGGTTTTTCTTCGGCCAGTCCGGCGCCGAGCCCCGG AGCCAATTGC	(SEQ ID NO:10)
20	L111A Sense	5'-GGGATTGGCGGCGCCGGACTGATCGAAG	(SEQ ID NO:11)
	Antisense	5'-CTTCGATCAGTCCGGCGCCGCAATCCC	(SEQ ID NO:12)
	F133A Sense	5'-GATCAGCCCATTCGCGGTACCGTCAACGATTGTG	(SEQ ID NO:13)
	Antisense	5'-CACAATCGTTGACGGTACCGCGAATGGGCTGATC	(SEQ ID NO:14)
25	I197A Sense	5'-GAGAAAGCCAGTACTCCGGCGGGCGTTGGTGG	(SEQ ID NO:15)
	Antisense	5'-CCACCAACGCCCGCCGGAGTACTGGCTTTCTC	(SEQ ID NO:16)

Example 3: Construct Preparation

3A. *E. coli* Expression Constructs

A series of constructs are prepared to direct the expression of the engineered KAS sequences in *E. coli*.

A series of constructs are prepared to direct the expression of the various engineered KAS sequences in host plant cells.

The construct pCGN10440 contains the I108F mutant expressed from the pQE30 (Qiagen) vector for expression in a host *E. coli* cell.

The construct pCGN10441 contains the I108L mutant expressed from the pQE30 (Qiagen) vector for expression in a host *E. coli* cell.

The construct pCGN10442 contains the A193I mutant expressed from the pQE30 (Qiagen) vector for expression in a host *E. coli* cell.

The construct pCGN10443 contains the I108F, A193I mutant expressed from the pQE30 (Qiagen) vector for expression in a host *E. coli* cell.

The construct pCGN10444 contains the I108L, A193I mutant expressed from the pQE30 (Qiagen) vector for expression in a host *E. coli* cell.

5 The construct pCGN10445 contains the A193M mutant expressed from the pQE30 (Qiagen) vector for expression in a host *E. coli* cell.

The construct pCGN10446 contains the I108F, A193M mutant expressed from the pQE30 (Qiagen) vector for expression in a host *E. coli* cell.

10 The construct pCGN10447 contains the I108L, A193M mutant expressed from the pQE30 (Qiagen) vector for expression in a host *E. coli* cell.

The construct pCGN10448 contains the L111A mutant expressed from the pQE30 (Qiagen) vector for expression in a host *E. coli* cell.

The construct pCGN10449 contains the F133A mutant expressed from the pQE30 (Qiagen) vector for expression in a host *E. coli* cell.

15 The construct pCGN10450 contains the L111A, F133A mutant expressed from the pQE30 (Qiagen) vector for expression in a host *E. coli* cell.

The construct pCGN10451 contains the I108A, L11A, I114A mutant expressed from the pQE30 (Qiagen) vector for expression in a host *E. coli* cell.

20 The construct pCGN10452 contains the F133A, L197A mutant expressed from the pQE30 (Qiagen) vector for expression in a host *E. coli* cell.

The construct pCGN10453 contains the I108A, L11A, I114A, F133A, L197A mutant expressed from the pQE30 (Qiagen) vector for expression in a host *E. coli* cell.

The construct pCGN10454 contains the L197A mutant expressed from the pQE30 (Qiagen) vector for expression in a host *E. coli* cell.

25

3B. Preparation of Plant Expression Constructs

A series of constructs are prepared to direct the expression of the engineered KAS sequences in plant host cells, both alone and in combination with additional sequences encoding proteins involved in fatty acid biosynthesis.

30

A plasmid containing the napin cassette derived from pCGN3223 (described in USPN 5,639,790, the entirety of which is incorporated herein by reference) was modified to make it more useful for cloning large DNA fragments containing multiple restriction sites, and to allow the cloning of multiple napin fusion genes into plant binary transformation vectors. An adapter comprised of the self annealed oligonucleotide of sequence
CGCGATTAAATGGCGCGCCCTGCAGGCGGCCGCTGCAGGGCGCGCCATTAAAT
(SEQ ID NO:) was ligated into the cloning vector pBC SK+ (Stratagene) after digestion with the restriction endonuclease BssHII to construct vector pCGN7765. Plasmids pCGN3223 and pCGN7765 were digested with NotI and ligated together. The resultant vector, pCGN7770, contains the pCGN7765 backbone with the napin seed specific expression cassette from pCGN3223.

A binary vector for plant transformation, pCGN5139, was constructed from pCGN1558 (McBride and Summerfelt, (1990) Plant Molecular Biology, 14:269-276). The polylinker of pCGN1558 was replaced as a HindIII/Asp718 fragment with a polylinker containing unique restriction endonuclease sites, AscI, PacI, XbaI, SwaI, BamHI, and NotI. The Asp718 and HindIII restriction endonuclease sites are retained in pCGN5139.

A binary vector, pCGN8642 was constructed to allow for the rapid cloning of various expression cassettes into the vector for use in plant transformation. The construct contains a multiple cloning region located between the right and left borders of the *Agrobacterium* transfer DNA. The construct also contains the Tn5 gene expressed from the 35S promoter between the multiple cloning site and the left border for selection of transformed plants on kanamycin.

A 354 bp BglII fragment containing the *Cuphea hookeriana* KASII-7 plastid targeting sequence (Figure 14) (SEQ ID NO:) was cloned into the BamHI site of the various pQE30 constructs containing the *E. coli* KASII (FabF) wild type or mutant KAS sequences. The resultant chimeric KAS II targeting sequence/FabF encoding sequence were cloned as HindIII/SalI fragments into filled-in SalI/XhoI sites of the napin expression cassette, pCGN7770. The resulting napin/KAS cassettes were cloned as NotI fragments into the NotI sites of various plant binary constructs as described below.

A napin cassette containing the coding sequence of the *Cuphea hookeriana* FatB2 protein (described in PCT Publication WO 98/46776, the entirety of which is incorporated herein by reference) was cloned as a *NotI* fragment into the *NotI* site of pCGN8642 to create pCGN11000.

A napin cassette containing the coding sequence of the *Garm FataI* protein (described in PCT Publication WO 97/12047, the entirety of which is incorporated herein by reference) was cloned into the *NotI* site of pCGN8642 to create pCGN11003.

A napin cassette containing the native (wild-type) *E. coli* KAS II coding sequence was cloned into the *NotI* site of pCGN11003 to create pCGN11040.

A napin cassette containing the native (wild-type) *E. coli* KAS II coding sequence was cloned into the *NotI* site of pCGN11003 to create pCGN11040.

A napin cassette containing the native (wild-type) *E. coli* KAS II coding sequence was cloned into the *NotI* site of pCGN8642 to create pCGN11041.

A napin cassette containing the native (wild-type) *E. coli* KAS II coding sequence was cloned into the *NotI* site of pCGN11000 to create pCGN11042.

A napin cassette containing the L111A KAS II mutant coding sequence was cloned into the *NotI* site of pCGN11003 to create pCGN11045.

A napin cassette containing the L111A KAS II mutant coding sequence was cloned into the *NotI* site of pCGN8642 to create pCGN11046.

A napin cassette containing the F133A KAS II mutant coding sequence was cloned into the *NotI* site of pCGN11003 to create pCGN11049.

A napin cassette containing the F133A KAS II mutant coding sequence was cloned into the *NotI* site of pCGN11003 to create pCGN11050.

A napin cassette containing the L111A, F133A KAS II double mutant coding sequence was cloned into the *NotI* site of pCGN11003 to create pCGN11053.

A napin cassette containing the L111A, F133A KAS II double mutant coding sequence was cloned into the *NotI* site of pCGN8642 to create pCGN11054.

A napin cassette containing the I108A, L111A, I114A KAS II triple mutant coding sequence was cloned into the *NotI* site of pCGN11003 to create pCGN11057.

A napin cassette containing the I108A, L111A, I114A KAS II triple mutant coding sequence was cloned into the *NotI* site of pCGN8642 to create pCGN11058.

A napin cassette containing the I108A, L111A, I114A, F133A, L197A KAS II multiple mutant coding sequence was cloned into the *NotI* site of pCGN11003 to create pCGN11061.

A napin cassette containing the I108A, L111A, I114A, F133A, L197A KAS II multiple mutant coding sequence was cloned into the *NotI* site of pCGN8642 to create pCGN11062.

5 A napin cassette containing the I108F KAS II mutant coding sequence was cloned into the *NotI* site of pCGN11000 to create pCGN11065.

A napin cassette containing the I108F KAS II mutant coding sequence was cloned into the *NotI* site of pCGN8642 to create pCGN11066.

10 A napin cassette containing the I108F, A193I KAS II double mutant coding sequence was cloned into the *NotI* site of pCGN11000 to create pCGN11069.

A napin cassette containing the I108F, A193I KAS II double mutant coding sequence was cloned into the *NotI* site of pCGN8642 to create pCGN11070.

A napin cassette containing the A193M KAS II mutant coding sequence was cloned into the *NotI* site of pCGN11000 to create pCGN11073.

15 A napin cassette containing the A193M KAS II mutant coding sequence was cloned into the *NotI* site of pCGN8642 to create pCGN11074.

Example 4: Analysis of Engineered KAS II Proteins Expression in *E. coli*

20 Figure 7 shows the complete list of mutations that were generated in *E.coli* KAS II using the Stratagene Quick-Change™ site-directed mutagenesis kit, and confirmed by DNA sequencing. The mutant KAS II genes cloned behind an IPTG inducible T5 promoter (pQE30 vector, Qiagen) were transformed into *E.coli* strain M15/pREP4. The effect of the expression of these KAS II mutants on the fatty acid composition of *E.coli* is shown in Figure 3. *E.coli* M15/pREP4 strains
25 containing no vector (-Vec), vector without insert (+Vec), or vectors expression wild-type KAS I or II or single or multiple engineered forms of KASII were grown to mid-log phase in LB media at 30°C. Expression was induced for 2 hours with IPTG (0.75 mM), cells were harvested, lyophilized, and the lipids were extracted into toluene and derivatized by sodium methoxide and analyzed for fatty acid content by GC FAME analysis as described in Dehesh, *et al.* (1998) *Plant*
30 *J.* 15:383-390.

The mutations prepared to increase the length of the end product fatty acids lead to the accumulation of abnormally long fatty acids in *E.coli* (Figure 3). Wild-type *E.coli* membranes contain no stearic acid and barely detectable levels of 20:0 and 20:1. Whereas L197, F133A and L111A all resulted in further elongation of the normal membrane components 16:0, and 18:1
5 resulting in the accumulation of 4, 7 and 13% 18:0 respectively, and 1 to 3% 20:0 and 20:1. KAS II/L111A produced the highest level of 18:0 (13%) while KAS II/L111A-F133A accumulated the highest levels of 20:0 and 20:1 (2 and 4% respectively). Mutations I108A and I114A appeared to decrease the long chain fatty acid accumulation due to L111A and F133A.

The KAS II mutants prepared to shorten the maximum fatty acids were analyzed *in vitro*
10 for the ability to utilize various chain length acyl-ACP substrates. Results of the *in vitro* assays (Figures 4, 5, and 6) demonstrates that the mutants I108F, I108L, A193M, and A193I have a reduced ability to utilize C8-ACP and longer substrates for condensation. However, these mutations are able to utilize C6-ACP substrates for elongation to produce C8 fatty acids. Furthermore, at least one mutation, A193M, had an increased ability to utilize C6-ACP substrates
15 compared to the wild-type KAS for elongation.

The data showing the effect of mutations I108F, I108L, A193I and A193M (together or separately) on the enzymatic activity of KAS II are summarized in figures 4, 5 and 6. Figure 4 shows that mutations I108F, I108L and A193M all cause significant reduction in the activity of KAS II on 8:0-ACP as compared to 6:0-ACP (38, 31 and 12 fold reductions respectively),
20 without significantly reducing the activity on 6:0-ACP. In other words they have effectively changed KAS II into an enzyme capable of making fatty acids up to a maximum of 8 carbons in length. Mutation A193I only causes a 1.8 fold decrease in activity on 8:0-ACP as compared to 6:0-ACP. Figure 5 shows that the combined mutations at I108 and A193 have the effect of reducing the activity of KAS II on 6:0-ACP somewhat, but figure 6 shows that the combined
25 effect was much greater effect on the activity with acyl-ACPs 8:0 and longer (14:0). Consequently the double mutants are even more specific for the synthesis of 8 carbon fatty acids. The most specific is KAS II I108F/A193 KAS II which is 90X more active on 6:0-ACP than it is on 8:0-ACP suggesting that it is now an enzyme highly specific for the synthesis of fatty acids only up to 8 carbons in length.

**Example 5: Structural Comparisons of a Plant Medium-Chain specific KAS
with *E.coli* KAS II**

To further characterize the structure-function relationships of KAS fatty acid binding pockets the modeled structure of a plant medium-chain (8:0, 10:0) specific KAS [*Cuphea. pulcherrima*, (*C.pu*) KASIV] (Dehesh *et al.* (1998) *Plant J.* 15:383-390) was compared with the crystal structure of *E.coli* KAS II. Figure 8 shows that *C.pu* KAS I is predicted to share essentially the same folding pattern as *E.coli* KAS II with the exception of a few loop regions, as might be expected given the structural similarity between KAS enzymes. Furthermore, *Cpu* KAS IV also has a similar structure (Figure 9). The general structure for the KAS family of proteins follows the α - β - α - β - α folding pattern. Indeed at the amino acid sequence level, all but 7 of the 55 highly conserved residues among KAS enzymes are identical (87% identity). However there is only 60% identity in hydrophobic fatty acid binding pocket region with 8 of the 20 amino acids being different consistent with this region of the protein being responsible for the differences in the enzymes specificity. Furthermore the model shows no steric hinderance in the formation of KASI and KASIV heterodimer (Figure 10). In addition, amino acid sequence comparisons between plant, mammalian, bacterial

Example 6: Plant Transformation and Analysis

The expression constructs described in Example 3B above were used to transform *Arabidopsis thaliana* (Columbia) and/or Columbia mutants *fab1*, *fae1-1*, and *fae1-2*.

Seeds from transformed *Arabidopsis* lines were analyzed for fatty acid composition and are provided in Table 2 below and shown in Figure 13. Fatty acid methyl esters (FAME) extracted in hexane were resolved by gas chromatography (GC) on a HewlettPackard model 6890 GC.

Table 2

Fatty Acid	12:0	14:0	16:0	16:1	18:0	18:1	18:1	18:2	18:3	20:0	20:1	20:1
	C9				C11				C13			
11058-AT002-19	0.29	0.17	7.86	0.50	3.85	14.53	3.37	26.02	18.72	2.83	11.61	3.71
11062-AT002-8	0.12	0.00	5.30	0.23	2.49	10.47	1.34	21.55	25.97	2.75	14.55	2.11
AT002-44	0.17	0.00	8.53	0.26	3.35	15.65	1.21	29.06	17.22	2.06	17.22	1.36
11041-AT002-9	0.00	0.00	9.46	0.29	3.49	13.87	1.18	27.32	18.88	2.28	17.52	1.43

Fatty Acid	20:2	20:3	22:0	22:1	22:2	22:3	24:0	24:1
11058-AT002-19	1.39	0.67	0.41	1.71	0.33	0.33	0.90	0.81
11062-AT002-8	2.56	2.07	0.55	5.36	0.40	1.13	0.42	0.63
AT002-44	1.63	0.36	0.29	1.26	0.02	0.07	0.14	0.14
11041-AT002-9	1.69	0.48	0.30	1.46	0.00	0.00	0.18	0.16

T2 pooled seeds from transgenic *Arabidopsis* lines containing pCGN11041 (11041-AT002-9) expressing the native *E. coli* KAS II protein in the seed tissue demonstrated nearly the same fatty acid composition as the nontransformed control *Arabidopsis* plants (AT002-44).

5 T2 pooled seeds from transgenic *Arabidopsis* var Columbia containing the construct pCGN11058 demonstrated the ability to synthesize longer carbon chain fatty acids compared to the nontransformed control plants as well as transgenic plants containing the wild-type *E. coli* KAS II protein. Particular increases in the production of 18:1 c11, 20:1 c13, 24:0 and 24:1 are observed in transgenic plants containing pCGN11058. Increases of 18:1 c11, 20:1 c13, 24:0 and 24:1 of 2 to 3 fold are obtained compared to nontransformed control plants. The fact that these
10 levels were not higher may be due to the fact that there are many enzymatic steps downstream from the condensation step catalyzed by KAS enzymes which affect the longer chain acyl-ACPs produced incorporation into triglycerides.

T2 pooled seeds from transgenic *Arabidopsis* var Columbia containing the construct pCGN11062 also demonstrated the ability to synthesize longer chain fatty acids compared to
15 nontransformed control plants and transgenic plants containing the wild-type *E. coli* KAS II protein construct. The T2 pooled seeds of 11062 transgenic lines were found to have a 3 to 4 fold increase in 22:1 as well as increased amounts of 20:2, 20:3 and 22:3, consistent with the presence of a KAS II protein being present in the plastid.

20 The above results demonstrate the ability to modify β -ketoacyl-ACP synthase sequences such that engineered β -ketoacyl-ACP synthases having altered substrate specificity may be produced. Such β -ketoacyl-ACP synthases may be expressed in host cells to provide a supply of the engineered β -ketoacyl-ACP synthase and to modify the existing pathway of fatty acid synthesis such that novel compositions of fatty acids are obtained. In particular, the engineered
25 β -ketoacyl-ACP synthases may be expressed in the seeds of oilseed plants to provide a natural source of desirable TAG molecules.

All publications and patent applications mentioned in this specification are indicative of the level of skill of those skilled in the art to which this invention pertains. All publications and
30 patent applications are herein incorporated by reference to the same extent as if each individual

publication or patent application was specifically and individually indicated to be incorporated by reference.

Although the foregoing invention has been described in some detail by way of illustration and example for purposes of clarity of understanding, it will be obvious that certain changes and
5 modifications may be practiced within the scope of the appended claims.

Claims

What is claimed is:

1. A method for obtaining an engineered β -ketoacyl-ACP synthase having an altered substrate
5 specificity with respect to the acyl-ACP substrates utilized by said β -ketoacyl-ACP synthase,
wherein said method comprises:
 - a) modifying a gene sequence encoding a first β -ketoacyl-ACP synthase protein to
produce a modified β -ketoacyl-ACP synthase gene sequence, wherein said modified
sequence encodes an engineered β -ketoacyl-ACP synthase having at least one
10 substitution, insertion or deletion of one or more amino acid residues in the mature
portion of said first β -ketoacyl-ACP synthase, and
 - b) expressing said modified gene sequence in a host cell, whereby said engineered β -
ketoacyl-ACP synthase is produced.
- 15 2. The method of claim 1 further comprising the step of assaying said engineered β -ketoacyl-
ACP synthase to detect altered substrate specificity.
3. The method according to claim 1 wherein said at least one amino acid substitution, insertion
or deletion is in a position selected from the group consisting of residue 105 - 120, 130 - 140,
20 190 - 200 and 340 - 400 of a β -ketoacyl-ACP synthase protein.
4. An amino acid sequence encoding a β -ketoacyl-ACP synthase protein wherein said sequence
has at least one substitution, insertion or deletion of at least one amino acid residue and said
protein has an altered substrate specificity.
- 25 5. The amino acid sequence of claim 4, wherein said amino acid sequence is obtained from a
prokaryotic source.

6. The amino acid sequence of claim 4, wherein said amino acid sequence is obtained from *E.coli*.
7. The amino acid sequence of claim 4, wherein said amino acid sequence is obtained from a plant source.
8. An amino acid sequence encoding a β -ketoacyl-ACP synthase protein wherein said sequence has at least one substitution, insertion or deletion of at least one amino acid residue selected from the group consisting of residue 105 - 120, 130 - 140, 190 - 205 and 340 - 400.
9. The amino acid sequence of claim 8, wherein said amino acid sequence is obtained from *E.coli*.
10. The amino acid sequence of claim 9 wherein said at least one amino acid substitution, insertion or deletion is in a position selected from the group consisting of residue 108, 111, 113, 114, 133, 138, 193, 197, and 203.
11. The amino acid sequence of claim 8, wherein said amino acid sequence is obtained from a plant source.
12. The amino acid sequence of claim 11 wherein said at least one amino acid substitution, insertion or deletion is in a position selected from the group consisting of residue 110, 113, 115, 116, 134, 139, 198, and 204.
13. A nucleic acid construct comprising as operably linked components in the 5' to 3' direction of transcription:
- a transcriptional initiation region; and
 - a polynucleotide sequence encoding a β -ketoacyl-ACP synthase having an altered substrate specificity.

14. The nucleic acid construct of claim 13, wherein said β -ketoacyl-ACP synthase has a engineered hydrophobic fatty acid binding pocket.

5 15. The nucleic acid construct of claim 13, wherein said β -ketoacyl-ACP synthase has been mutated in a region corresponding to an amino acid selected from the group consisting of residue 105 - 120, 130 - 140, 190 - 200 and 340 - 400.

16. A method for altering the fatty acid composition of a host cell comprising;

10 transforming a host cell with a nucleic acid expression construct comprising a transcription initiation region, and a nucleic acid sequence encoding a β -ketoacyl-ACP synthase having altered substrate specificity, and
growing said host cell under appropriate culture conditions such that the fatty acid composition is altered in said host cell.

15

**ENGINEERING β -KETOACYL ACP SYNTHASE HAVING NOVEL SUBSTRATE
SPECIFICITY**

5

ABSTRACT

Methods of altering substrate specificity of beta-ketoacyl-ACP synthase, and engineered beta-ketoacyl-ACP synthases so produced are provided. DNA sequences and constructs for expression of engineered beta-ketoacyl-ACP synthases, as well as the novel beta-ketoacyl-ACP synthases produced therefrom are also provided. Such DNA sequences may be used for expression of the engineered beta-ketoacyl-ACP synthases in host cells, particularly seed cells of oilseed crop plants, for the modification of fatty acid composition.

10

CB	LYS	A	2	5.613	-3.324	2.834	1.00	59.14	6
C	LYS	A	2	6.322	-2.753	4.050	1.00	61.37	6
C	LYS	A	2	5.431	-1.783	4.810	1.00	63.79	6
CE	LYS	A	2	5.988	-0.370	4.758	1.00	65.75	6
NZ	LYS	A	2	6.107	0.235	6.114	1.00	67.05	7
C	LYS	A	2	7.506	-2.721	1.297	1.00	54.28	6
O	LYS	A	2	8.092	-3.798	1.180	1.00	55.04	8
N	LYS	A	2	5.283	-3.329	0.369	1.00	55.75	7
CA	LYS	A	2	5.997	-2.678	1.505	1.00	55.55	6
N	ARG	A	3	8.133	-1.550	1.248	1.00	51.95	7
CA	ARG	A	3	9.568	-1.460	1.019	1.00	49.09	6
CB	ARG	A	3	9.832	-0.701	-0.286	1.00	45.74	6
C	ARG	A	3	9.634	-1.551	-1.531	1.00	42.70	6
C	ARG	A	3	9.283	-0.696	-2.736	1.00	39.77	6
N	ARG	A	3	10.401	0.132	-3.168	1.00	37.67	7
CZ	ARG	A	3	11.302	-0.211	-4.077	1.00	38.43	6
N	ARG	A	3	11.252	-1.395	-4.674	1.00	36.91	7
N	ARG	A	3	12.270	0.640	-4.395	1.00	39.50	7
C	ARG	A	3	10.314	-0.795	2.167	1.00	47.74	6
O	ARG	A	3	10.086	0.368	2.498	1.00	48.18	8
N	ARG	A	4	11.236	-1.548	2.759	1.00	45.69	7
CA	ARG	A	4	12.030	-1.079	3.884	1.00	43.14	6
CB	ARG	A	4	12.459	-2.265	4.753	1.00	45.59	6
C	ARG	A	4	11.299	-3.046	5.351	1.00	49.39	6
C	ARG	A	4	11.719	-4.453	5.750	1.00	52.07	6
N	ARG	A	4	12.975	-4.463	6.482	1.00	56.09	7
CZ	ARG	A	4	13.402	-5.394	7.320	1.00	57.45	6
N	ARG	A	4	12.671	-6.469	7.583	1.00	58.72	7
N	ARG	A	4	14.583	-5.250	7.911	1.00	58.03	7
C	ARG	A	4	13.258	-0.297	3.435	1.00	40.93	6
O	ARG	A	4	13.873	-0.605	2.416	1.00	40.28	8
N	VAL	A	5	13.590	0.744	4.194	1.00	38.82	7
CA	VAL	A	5	14.729	1.598	3.891	1.00	37.38	6
CB	VAL	A	5	14.346	3.087	3.796	1.00	36.10	6
C	VAL	A	5	15.533	3.916	3.320	1.00	33.72	6
C	VAL	A	5	13.154	3.308	2.877	1.00	36.27	6
C	VAL	A	5	15.816	1.453	4.953	1.00	36.82	6
O	VAL	A	5	15.549	1.542	6.151	1.00	36.76	8
N	VAL	A	6	17.046	1.229	4.506	1.00	36.09	7
CA	VAL	A	6	18.188	1.076	5.394	1.00	35.35	6
CB	VAL	A	6	18.784	-0.343	5.351	1.00	34.87	6
C	VAL	A	6	17.864	-1.358	6.013	1.00	34.92	6
C	VAL	A	6	19.087	-0.767	3.921	1.00	33.83	6
C	VAL	A	6	19.280	2.084	5.044	1.00	35.02	6
O	VAL	A	6	19.291	2.649	3.954	1.00	34.67	8
N	VAL	A	7	20.190	2.324	5.981	1.00	35.45	7
CA	VAL	A	7	21.298	3.256	5.781	1.00	34.76	6
CB	VAL	A	7	21.519	4.143	7.016	1.00	34.20	6
C	VAL	A	7	22.549	5.229	6.736	1.00	35.28	6
C	VAL	A	7	20.207	4.769	7.474	1.00	33.35	6
C	VAL	A	7	22.567	2.474	5.464	1.00	34.53	6
O	VAL	A	7	23.042	1.691	6.287	1.00	34.58	8
N	THR	A	8	23.109	2.663	4.264	1.00	34.21	7
CA	THR	A	8	24.292	1.941	3.833	1.00	33.29	6
CB	THR	A	8	24.005	1.203	2.496	1.00	32.59	6
O	THR	A	8	23.817	2.189	1.470	1.00	33.02	8
C	THR	A	8	22.787	0.308	2.579	1.00	29.02	6
C	THR	A	8	25.539	2.774	3.600	1.00	33.18	6
O	THR	A	8	26.490	2.253	3.004	1.00	33.39	8
N	GLY	A	9	25.560	4.034	4.005	1.00	33.20	7
CA	GLY	A	9	26.733	4.875	3.757	1.00	32.15	6
C	GLY	A	9	26.610	6.183	4.528	1.00	31.83	6
O	GLY	A	9	25.543	6.795	4.564	1.00	30.94	8
N	LEU	A	1	27.702	6.580	5.174	1.00	31.18	7

CA	LEU	A	1	27.715	7.796	5.976	1.00	30.88	6
CB	LEU	A	1	27.832	7.470	7.465	1.00	30.95	6
C	LEU	A	1	26.817	6.517	8.091	1.00	31.61	6
C	LEU	A	1	27.194	6.187	9.528	1.00	32.70	6
C	LEU	A	1	25.410	7.097	8.027	1.00	30.96	6
C	LEU	A	1	28.867	8.701	5.557	1.00	30.32	6
O	LEU	A	1	29.922	8.221	5.142	1.00	31.20	8
N	GLY	A	1	28.660	10.006	5.668	1.00	29.75	7
CA	GLY	A	1	29.701	10.970	5.306	1.00	29.27	6
C	GLY	A	1	29.422	12.296	6.007	1.00	28.70	6
O	GLY	A	1	28.260	12.602	6.284	1.00	28.60	8
N	MET	A	1	30.471	13.052	6.317	1.00	28.95	7
CA	MET	A	1	30.279	14.332	6.974	1.00	28.89	6
CB	MET	A	1	29.500	14.156	8.282	1.00	31.91	6
C	MET	A	1	30.318	14.051	9.554	1.00	34.60	6
SD	MET	A	1	29.290	14.107	11.033	1.00	35.65	1
CE	MET	A	1	29.116	12.360	11.381	1.00	37.75	6
C	MET	A	1	31.547	15.130	7.258	1.00	28.38	6
O	MET	A	1	32.668	14.671	7.402	1.00	27.81	8
N	LEU	A	1	31.299	16.426	7.387	1.00	27.53	7
CA	LEU	A	1	32.257	17.446	7.762	1.00	27.49	6
CB	LEU	A	1	32.577	18.409	6.630	1.00	29.94	6
C	LEU	A	1	33.334	17.830	5.431	1.00	32.91	6
C	LEU	A	1	33.043	18.630	4.173	1.00	33.46	6
C	LEU	A	1	34.828	17.784	5.721	1.00	33.17	6
C	LEU	A	1	31.597	18.185	8.933	1.00	27.03	6
O	LEU	A	1	30.438	18.586	8.823	1.00	26.86	8
N	SER	A	1	32.312	18.320	10.034	1.00	27.31	7
CA	SER	A	1	31.761	18.998	11.205	1.00	28.03	6
CB	SER	A	1	31.153	17.968	12.155	1.00	28.80	6
O	SER	A	1	32.095	17.519	13.112	1.00	31.76	8
C	SER	A	1	32.860	19.787	11.895	1.00	28.55	6
O	SER	A	1	34.043	19.612	11.612	1.00	28.57	8
N	PRO	A	1	32.488	20.594	12.880	1.00	29.49	7
C	PRO	A	1	31.084	20.865	13.288	1.00	29.61	6
CA	PRO	A	1	33.426	21.371	13.665	1.00	29.78	6
CB	PRO	A	1	32.547	22.264	14.535	1.00	29.65	6
C	PRO	A	1	31.201	22.240	13.902	1.00	29.56	6
C	PRO	A	1	34.379	20.543	14.509	1.00	30.22	6
O	PRO	A	1	35.409	21.090	14.924	1.00	30.34	8
N	VAL	A	1	34.099	19.277	14.817	1.00	30.78	7
CA	VAL	A	1	35.023	18.464	15.592	1.00	31.66	6
CB	VAL	A	1	34.400	17.804	16.836	1.00	31.11	6
C	VAL	A	1	34.067	18.850	17.890	1.00	32.88	6
C	VAL	A	1	33.175	16.980	16.477	1.00	31.36	6
C	VAL	A	1	35.695	17.376	14.761	1.00	32.04	6
O	VAL	A	1	36.346	16.500	15.340	1.00	33.52	8
N	GLY	A	1	35.563	17.410	13.440	1.00	31.84	7
CA	GLY	A	1	36.197	16.390	12.612	1.00	31.47	6
C	GLY	A	1	35.809	16.494	11.146	1.00	31.36	6
O	GLY	A	1	34.696	16.904	10.817	1.00	31.58	8
N	ASN	A	1	36.727	16.101	10.269	1.00	30.64	7
CA	ASN	A	1	36.512	16.147	8.833	1.00	30.14	6
CB	ASN	A	1	37.798	16.560	8.113	1.00	35.19	6
C	ASN	A	1	37.969	18.057	7.977	1.00	40.02	6
O	ASN	A	1	37.973	18.798	8.961	1.00	43.84	8
N	ASN	A	1	38.133	18.535	6.748	1.00	43.10	7
C	ASN	A	1	36.017	14.824	8.269	1.00	29.28	6
O	ASN	A	1	35.843	14.691	7.058	1.00	28.86	8
N	THR	A	1	35.881	13.805	9.104	1.00	29.33	7
CA	THR	A	1	35.345	12.514	8.721	1.00	28.83	6
CB	THR	A	1	36.381	11.377	8.653	1.00	27.69	6
O	THR	A	1	37.050	11.283	9.920	1.00	29.59	8
C	THR	A	1	37.397	11.575	7.548	1.00	25.58	6

Figure 1 - 1

N	LYS	A	5	37.449	23.043	10.349	1.00	36.41	7
CA	LYS	A	5	38.878	23.314	10.391	1.00	38.50	6
CB	LYS	A	5	39.363	23.117	11.840	1.00	38.42	6
C	LYS	A	5	38.814	24.167	12.794	1.00	40.28	6
CE	LYS	A	5	38.770	23.668	14.228	1.00	42.84	6
C	LYS	A	5	37.350	23.437	14.705	1.00	43.44	6
NZ	LYS	A	5	36.653	24.697	15.081	1.00	44.14	7
C	LYS	A	5	39.718	22.478	9.444	1.00	40.42	6
O	LYS	A	5	39.596	21.260	9.337	1.00	40.62	8
N	ASP	A	5	40.664	23.147	8.783	1.00	42.10	7
CA	ASP	A	5	41.617	22.514	7.881	1.00	43.84	6
CB	ASP	A	5	42.512	21.555	8.678	1.00	47.61	6
C	ASP	A	5	43.289	22.268	9.771	1.00	50.56	6
O	ASP	A	5	43.952	23.279	9.459	1.00	52.38	8
O	ASP	A	5	43.187	21.836	10.940	1.00	52.15	8
C	ASP	A	5	40.941	21.788	6.727	1.00	44.21	6
O	ASP	A	5	41.227	20.626	6.428	1.00	44.58	8
N	PHE	A	5	40.050	22.488	6.037	1.00	43.94	7
CA	PHE	A	5	39.275	21.914	4.945	1.00	44.27	6
CB	PHE	A	5	37.963	22.698	4.825	1.00	38.90	6
C	PHE	A	5	37.060	22.308	3.696	1.00	34.96	6
C	PHE	A	5	36.432	21.075	3.672	1.00	32.24	6
C	PHE	A	5	36.827	23.193	2.653	1.00	33.21	6
CE	PHE	A	5	35.597	20.725	2.629	1.00	31.61	6
CE	PHE	A	5	35.992	22.848	1.607	1.00	32.75	6
CZ	PHE	A	5	35.377	21.612	1.595	1.00	32.24	6
C	PHE	A	5	40.028	21.868	3.627	1.00	45.76	6
O	PHE	A	5	40.511	22.875	3.115	1.00	45.77	8
N	ASN	A	5	40.109	20.672	3.051	1.00	47.93	7
CA	ASN	A	5	40.764	20.458	1.769	1.00	50.19	6
CB	ASN	A	5	42.108	19.750	1.930	1.00	55.16	6
C	ASN	A	5	42.893	19.657	0.637	1.00	59.33	6
O	ASN	A	5	43.373	18.585	0.266	1.00	61.85	8
N	ASN	A	5	43.038	20.776	-0.065	1.00	60.64	7
C	ASN	A	5	39.860	19.647	0.842	1.00	50.97	6
O	ASN	A	5	39.380	18.573	1.203	1.00	51.24	8
N	CYS	A	5	39.606	20.198	-0.338	1.00	51.32	7
CA	CYS	A	5	38.762	19.529	-1.322	1.00	52.14	6
CB	CYS	A	5	37.365	20.144	-1.347	1.00	52.43	6
SG	CYS	A	5	37.309	21.830	-1.997	1.00	50.96	1
C	CYS	A	5	39.408	19.600	-2.699	1.00	52.89	6
O	CYS	A	5	38.805	19.251	-3.709	1.00	52.44	8
N	GLU	A	5	40.689	19.951	-2.722	1.00	54.30	7
CA	GLU	A	5	41.479	20.027	-3.943	1.00	56.17	6
CB	GLU	A	5	42.919	20.418	-3.604	1.00	60.28	6
C	GLU	A	5	43.697	21.045	-4.743	1.00	65.46	6
C	GLU	A	5	43.878	22.543	-4.612	1.00	68.19	6
O	GLU	A	5	44.798	23.084	-5.266	1.00	69.51	8
O	GLU	A	5	43.111	23.192	-3.872	1.00	69.64	8
C	GLU	A	5	41.457	18.714	-4.717	1.00	56.61	6
O	GLU	A	5	41.277	18.697	-5.936	1.00	56.60	8
N	ASP	A	6	41.571	17.594	-4.013	1.00	57.07	7
CA	ASP	A	6	41.491	16.269	-4.601	1.00	57.64	6
CB	ASP	A	6	41.873	15.183	-3.599	1.00	62.92	6
C	ASP	A	6	41.772	15.563	-2.141	1.00	66.58	6
O	ASP	A	6	40.916	14.989	-1.431	1.00	68.82	8
O	ASP	A	6	42.559	16.417	-1.677	1.00	68.78	8
C	ASP	A	6	40.111	15.977	-5.186	1.00	56.94	6
O	ASP	A	6	40.014	15.332	-6.232	1.00	56.79	8
N	ILE	A	6	39.049	16.432	-4.531	1.00	56.25	7
CA	ILE	A	6	37.691	16.200	-4.995	1.00	55.48	6
CB	ILE	A	6	36.685	16.184	-3.824	1.00	54.74	6
C	ILE	A	6	35.366	15.567	-4.270	1.00	53.87	6
C	ILE	A	6	37.242	15.462	-2.600	1.00	54.58	6

C	ILE	A	6	37.567	13.998	-2.774	1.00	54.63	6
C	ILE	A	6	37.223	17.225	-6.020	1.00	55.26	6
O	ILE	A	6	36.583	16.871	-7.013	1.00	54.72	8
N	ILE	A	6	37.389	18.509	-5.720	1.00	55.58	7
CA	ILE	A	6	36.959	19.594	-6.587	1.00	56.21	6
CB	ILE	A	6	35.885	20.502	-5.963	1.00	54.72	6
C	ILE	A	6	35.379	21.516	-6.985	1.00	53.62	6
C	ILE	A	6	34.697	19.717	-5.404	1.00	54.25	6
C	ILE	A	6	34.399	20.027	-3.952	1.00	53.74	6
C	ILE	A	6	38.151	20.477	-6.962	1.00	57.36	6
O	ILE	A	6	38.886	20.940	-6.089	1.00	56.79	8
N	SER	A	6	38.297	20.751	-8.254	1.00	59.16	7
CA	SER	A	6	39.409	21.565	-8.732	1.00	61.00	6
CB	SER	A	6	39.496	21.520	-10.258	1.00	61.46	6
O	SER	A	6	38.215	21.648	-10.849	1.00	63.02	8
C	SER	A	6	39.286	23.007	-8.261	1.00	62.26	6
O	SER	A	6	38.203	23.459	-7.890	1.00	62.61	8
N	ARG	A	6	40.389	23.749	-8.340	1.00	63.24	7
CA	ARG	A	6	40.391	25.163	-7.975	1.00	64.33	6
CB	ARG	A	6	41.798	25.733	-7.862	1.00	70.36	6
C	ARG	A	6	42.847	24.781	-7.312	1.00	75.55	6
C	ARG	A	6	43.965	24.570	-8.322	1.00	79.64	6
N	ARG	A	6	44.571	23.249	-8.210	1.00	83.48	7
CZ	ARG	A	6	45.874	23.006	-8.289	1.00	85.63	6
N	ARG	A	6	46.737	23.996	-8.481	1.00	87.20	7
N	ARG	A	6	46.327	21.764	-8.173	1.00	86.70	7
C	ARG	A	6	39.578	25.952	-9.003	1.00	63.68	6
O	ARG	A	6	38.912	26.929	-8.665	1.00	63.91	8
N	LYS	A	6	39.621	25.512	-10.259	1.00	62.41	7
CA	LYS	A	6	38.838	26.122	-11.323	1.00	61.01	6
CB	LYS	A	6	39.078	25.442	-12.667	1.00	64.05	6
C	LYS	A	6	40.473	25.584	-13.247	1.00	67.89	6
C	LYS	A	6	40.692	24.601	-14.390	1.00	70.27	6
CE	LYS	A	6	42.115	24.069	-14.405	1.00	72.41	6
NZ	LYS	A	6	42.174	22.613	-14.094	1.00	73.35	7
C	LYS	A	6	37.355	25.994	-10.959	1.00	59.05	6
O	LYS	A	6	36.623	26.977	-10.893	1.00	59.16	8
N	GLU	A	6	36.933	24.768	-10.663	1.00	56.50	7
CA	GLU	A	6	35.560	24.458	-10.303	1.00	54.00	6
CB	GLU	A	6	35.351	22.937	-10.348	1.00	53.27	6
C	GLU	A	6	35.135	22.410	-11.759	1.00	52.23	6
C	GLU	A	6	33.753	22.724	-12.296	1.00	51.74	6
O	GLU	A	6	33.652	23.202	-13.444	1.00	49.51	8
O	GLU	A	6	32.764	22.494	-11.571	1.00	52.67	8
C	GLU	A	6	35.113	25.008	-8.961	1.00	52.28	6
O	GLU	A	6	33.929	25.285	-8.749	1.00	51.71	8
N	GLN	A	6	36.032	25.227	-8.034	1.00	50.86	7
CA	GLN	A	6	35.780	25.773	-6.715	1.00	49.27	6
CB	GLN	A	6	37.107	25.821	-5.948	1.00	49.56	6
C	GLN	A	6	37.061	25.384	-4.497	1.00	50.72	6
C	GLN	A	6	38.460	25.262	-3.918	1.00	51.56	6
O	GLN	A	6	39.130	26.269	-3.682	1.00	51.87	8
N	GLN	A	6	38.908	24.031	-3.700	1.00	50.91	7
C	GLN	A	6	35.184	27.173	-6.731	1.00	48.26	6
O	GLN	A	6	34.447	27.566	-5.825	1.00	48.39	8
N	ARG	A	6	35.475	27.960	-7.756	1.00	47.26	7
CA	ARG	A	6	35.017	29.320	-7.939	1.00	45.38	6
CB	ARG	A	6	35.835	29.966	-9.074	1.00	52.16	6
C	ARG	A	6	35.884	31.480	-9.005	1.00	59.18	6
C	ARG	A	6	35.460	32.120	-10.317	1.00	65.00	6
N	ARG	A	6	34.851	33.429	-10.120	1.00	70.09	7
CZ	ARG	A	6	35.477	34.531	-9.730	1.00	72.67	6
N	ARG	A	6	36.780	34.518	-9.476	1.00	73.94	7
N	ARG	A	6	34.797	35.664	-9.589	1.00	74.21	7

Figure 1 - 4

C	ARG	A	6	33.541	29.463	-8.272	1.00	42.38	6
O	ARG	A	6	32.974	30.555	-8.163	1.00	42.43	8
N	LYS	A	6	32.895	28.387	-8.698	1.00	38.98	7
CA	LYS	A	6	31.489	28.391	-9.047	1.00	36.08	6
CB	LYS	A	6	31.233	27.425	-10.211	1.00	38.25	6
C	LYS	A	6	32.187	27.547	-11.385	1.00	41.26	6
C	LYS	A	6	31.832	26.533	-12.467	1.00	43.21	6
CE	LYS	A	6	32.688	26.729	-13.707	1.00	45.12	6
NZ	LYS	A	6	32.841	25.473	-14.491	1.00	44.54	7
C	LYS	A	6	30.595	27.970	-7.885	1.00	33.41	6
O	LYS	A	6	29.393	27.786	-8.094	1.00	32.34	8
N	MET	A	7	31.148	27.782	-6.690	1.00	31.31	7
CA	MET	A	7	30.352	27.276	-5.584	1.00	30.21	6
CB	MET	A	7	30.475	25.744	-5.527	1.00	32.32	6
C	MET	A	7	31.857	25.194	-5.822	1.00	35.12	6
SD	MET	A	7	31.957	23.402	-5.704	1.00	36.02	1
CE	MET	A	7	31.529	22.901	-7.367	1.00	34.53	6
C	MET	A	7	30.684	27.848	-4.215	1.00	28.31	6
O	MET	A	7	31.832	27.922	-3.787	1.00	28.11	8
N	ASP	A	7	29.624	28.234	-3.503	1.00	25.95	7
CA	ASP	A	7	29.766	28.751	-2.143	1.00	23.65	6
CB	ASP	A	7	28.413	29.222	-1.616	1.00	20.66	6
C	ASP	A	7	28.479	29.865	-0.246	1.00	22.27	6
O	ASP	A	7	28.312	29.143	0.762	1.00	21.88	8
O	ASP	A	7	28.718	31.089	-0.170	1.00	21.04	8
C	ASP	A	7	30.326	27.629	-1.273	1.00	22.62	6
O	ASP	A	7	30.144	26.453	-1.603	1.00	22.32	8
N	ALA	A	7	30.882	27.953	-0.115	1.00	21.68	7
CA	ALA	A	7	31.389	26.979	0.831	1.00	21.95	6
CB	ALA	A	7	31.922	27.690	2.079	1.00	19.90	6
C	ALA	A	7	30.380	25.920	1.251	1.00	22.22	6
O	ALA	A	7	30.796	24.777	1.483	1.00	22.29	8
N	PHE	A	7	29.093	26.236	1.373	1.00	22.19	7
CA	PHE	A	7	28.095	25.239	1.753	1.00	22.22	6
CB	PHE	A	7	26.728	25.848	2.038	1.00	20.07	6
C	PHE	A	7	25.717	25.891	0.936	1.00	17.46	6
C	PHE	A	7	24.749	24.907	0.811	1.00	18.74	6
C	PHE	A	7	25.726	26.918	0.006	1.00	17.25	6
CE	PHE	A	7	23.818	24.946	-0.210	1.00	18.48	6
CE	PHE	A	7	24.806	26.962	-1.024	1.00	12.10	6
CZ	PHE	A	7	23.842	25.981	-1.126	1.00	15.15	6
C	PHE	A	7	28.014	24.132	0.705	1.00	22.32	6
O	PHE	A	7	27.900	22.958	1.064	1.00	22.55	8
N	ILE	A	7	28.084	24.484	-0.574	1.00	22.33	7
CA	ILE	A	7	28.084	23.492	-1.645	1.00	22.84	6
CB	ILE	A	7	27.881	24.146	-3.022	1.00	23.95	6
C	ILE	A	7	28.144	23.175	-4.164	1.00	24.20	6
C	ILE	A	7	26.451	24.694	-3.121	1.00	21.72	6
C	ILE	A	7	26.260	25.703	-4.232	1.00	20.39	6
C	ILE	A	7	29.365	22.667	-1.611	1.00	22.04	6
O	ILE	A	7	29.318	21.448	-1.777	1.00	20.83	8
N	GLN	A	7	30.501	23.312	-1.364	1.00	22.64	7
CA	GLN	A	7	31.777	22.612	-1.257	1.00	23.44	6
CB	GLN	A	7	32.923	23.597	-1.047	1.00	25.82	6
C	GLN	A	7	33.158	24.544	-2.211	1.00	29.28	6
C	GLN	A	7	34.326	25.483	-1.984	1.00	31.36	6
O	GLN	A	7	35.184	25.241	-1.131	1.00	33.44	8
N	GLN	A	7	34.369	26.565	-2.755	1.00	28.85	7
C	GLN	A	7	31.730	21.592	-0.122	1.00	23.75	6
O	GLN	A	7	32.095	20.428	-0.314	1.00	24.15	8
N	TYR	A	7	31.209	21.984	1.038	1.00	23.05	7
CA	TYR	A	7	31.025	21.063	2.151	1.00	23.66	6
CB	TYR	A	7	30.436	21.773	3.365	1.00	23.91	6
C	TYR	A	7	31.303	22.775	4.083	1.00	24.75	6

C	TYR	A	7	30.779	23.481	5.163	1.00	25.10	6
CE	TYR	A	7	31.538	24.408	5.853	1.00	25.02	6
C	TYR	A	7	32.615	23.038	3.717	1.00	25.66	6
CE	TYR	A	7	33.382	23.970	4.390	1.00	25.67	6
CZ	TYR	A	7	32.835	24.651	5.457	1.00	25.21	6
O	TYR	A	7	33.592	25.576	6.133	1.00	25.47	8
C	TYR	A	7	30.106	19.904	1.768	1.00	23.62	6
O	TYR	A	7	30.406	18.741	2.037	1.00	23.40	8
N	GLY	A	7	28.986	20.218	1.124	1.00	22.96	7
CA	GLY	A	7	28.018	19.230	0.696	1.00	23.75	6
C	GLY	A	7	28.588	18.158	-0.218	1.00	24.27	6
O	GLY	A	7	28.290	16.977	-0.034	1.00	23.78	8
N	ILE	A	7	29.369	18.551	-1.219	1.00	25.10	7
CA	ILE	A	7	29.975	17.602	-2.144	1.00	25.73	6
CB	ILE	A	7	30.674	18.315	-3.316	1.00	27.05	6
C	ILE	A	7	31.383	17.316	-4.222	1.00	27.14	6
C	ILE	A	7	29.645	19.119	-4.117	1.00	27.25	6
C	ILE	A	7	30.230	20.052	-5.152	1.00	29.01	6
C	ILE	A	7	30.945	16.669	-1.430	1.00	25.57	6
O	ILE	A	7	30.797	15.447	-1.504	1.00	24.87	8
N	VAL	A	7	31.896	17.231	-0.691	1.00	25.62	7
CA	VAL	A	7	32.878	16.438	0.045	1.00	25.35	6
CB	VAL	A	7	33.812	17.327	0.881	1.00	22.69	6
C	VAL	A	7	34.663	16.522	1.851	1.00	21.61	6
C	VAL	A	7	34.714	18.139	-0.045	1.00	22.34	6
C	VAL	A	7	32.199	15.387	0.909	1.00	26.06	6
O	VAL	A	7	32.502	14.198	0.786	1.00	27.16	8
N	ALA	A	8	31.232	15.783	1.731	1.00	26.43	7
CA	ALA	A	8	30.483	14.846	2.558	1.00	26.69	6
CB	ALA	A	8	29.549	15.590	3.500	1.00	25.12	6
C	ALA	A	8	29.689	13.857	1.711	1.00	27.31	6
O	ALA	A	8	29.503	12.707	2.112	1.00	26.33	8
N	GLY	A	8	29.198	14.295	0.555	1.00	28.24	7
CA	GLY	A	8	28.478	13.434	-0.370	1.00	29.83	6
C	GLY	A	8	29.401	12.376	-0.965	1.00	31.54	6
O	GLY	A	8	29.058	11.195	-1.014	1.00	32.46	8
N	VAL	A	8	30.606	12.785	-1.357	1.00	32.13	7
CA	VAL	A	8	31.593	11.855	-1.897	1.00	32.49	6
CB	VAL	A	8	32.849	12.576	-2.405	1.00	32.48	6
C	VAL	A	8	33.927	11.590	-2.836	1.00	29.55	6
C	VAL	A	8	32.485	13.493	-3.570	1.00	30.84	6
C	VAL	A	8	31.945	10.798	-0.859	1.00	33.38	6
O	VAL	A	8	31.960	9.607	-1.179	1.00	34.11	8
N	GLN	A	8	32.121	11.195	0.397	1.00	33.20	7
CA	GLN	A	8	32.353	10.260	1.485	1.00	33.16	6
CB	GLN	A	8	32.487	10.995	2.822	1.00	33.36	6
C	GLN	A	8	33.776	11.775	3.007	1.00	34.15	6
C	GLN	A	8	33.891	12.385	4.389	1.00	35.18	6
O	GLN	A	8	33.162	12.014	5.309	1.00	35.45	8
N	GLN	A	8	34.810	13.330	4.554	1.00	35.50	7
C	GLN	A	8	31.240	9.224	1.602	1.00	33.48	6
O	GLN	A	8	31.521	8.034	1.758	1.00	33.91	8
N	ALA	A	8	29.982	9.655	1.539	1.00	33.54	7
CA	ALA	A	8	28.854	8.740	1.660	1.00	33.80	6
CB	ALA	A	8	27.554	9.509	1.828	1.00	32.23	6
C	ALA	A	8	28.767	7.777	0.484	1.00	34.48	6
O	ALA	A	8	28.464	6.596	0.673	1.00	34.17	8
N	MET	A	8	29.032	8.262	-0.724	1.00	35.38	7
CA	MET	A	8	29.047	7.401	-1.902	1.00	36.89	6
CB	MET	A	8	29.234	8.228	-3.172	1.00	39.17	6
C	MET	A	8	27.977	8.960	-3.621	1.00	41.02	6
SD	MET	A	8	26.540	7.880	-3.753	1.00	43.01	1
CE	MET	A	8	26.317	7.818	-5.528	1.00	43.92	6
C	MET	A	8	30.132	6.340	-1.757	1.00	37.28	6

Figure 1 - 5

O	MET	A	8	29.873	5.147	-1.919	1.00	37.28	8
N	GLN	A	8	31.338	6.765	-1.397	1.00	37.87	7
CA	GLN	A	8	32.462	5.860	-1.192	1.00	38.47	6
CB	GLN	A	8	33.741	6.661	-0.925	1.00	39.65	6
C	GLN	A	8	34.320	7.292	-2.182	1.00	41.26	6
C	GLN	A	8	35.553	8.126	-1.924	1.00	44.46	6
O	GLN	A	8	35.965	8.328	-0.781	1.00	48.85	8
N	GLN	A	8	36.170	8.625	-2.991	1.00	45.09	7
C	GLN	A	8	32.195	4.862	-0.077	1.00	38.33	6
O	GLN	A	8	32.309	3.653	-0.293	1.00	38.79	8
N	ASP	A	8	31.705	5.316	1.071	1.00	38.25	7
CA	ASP	A	8	31.356	4.431	2.171	1.00	38.61	6
CB	ASP	A	8	30.800	5.221	3.364	1.00	35.92	6
C	ASP	A	8	30.769	4.381	4.627	1.00	34.86	6
O	ASP	A	8	31.730	3.609	4.836	1.00	38.15	8
O	ASP	A	8	29.807	4.473	5.413	1.00	32.47	8
C	ASP	A	8	30.338	3.362	1.785	1.00	39.15	6
O	ASP	A	8	30.418	2.228	2.261	1.00	39.15	8
N	SER	A	8	29.341	3.717	0.987	1.00	40.00	7
CA	SER	A	8	28.268	2.824	0.605	1.00	40.96	6
CB	SER	A	8	27.186	3.609	-0.151	1.00	37.71	6
O	SER	A	8	27.641	3.995	-1.435	1.00	34.05	8
C	SER	A	8	28.687	1.626	-0.235	1.00	42.86	6
O	SER	A	8	28.158	0.529	-0.031	1.00	42.42	8
N	GLY	A	8	29.572	1.835	-1.203	1.00	44.78	7
CA	GLY	A	8	29.933	0.745	-2.114	1.00	47.74	6
C	GLY	A	8	28.791	0.593	-3.124	1.00	49.79	6
O	GLY	A	8	28.100	-0.420	-3.181	1.00	50.71	8
N	LEU	A	9	28.528	1.689	-3.826	1.00	51.03	7
CA	LEU	A	9	27.506	1.717	-4.861	1.00	52.32	6
CB	LEU	A	9	26.528	2.868	-4.677	1.00	54.13	6
C	LEU	A	9	25.057	2.570	-4.394	1.00	54.85	6
C	LEU	A	9	24.486	1.519	-5.334	1.00	54.50	6
C	LEU	A	9	24.866	2.145	-2.943	1.00	55.70	6
C	LEU	A	9	28.206	1.842	-6.216	1.00	53.14	6
O	LEU	A	9	29.081	2.691	-6.384	1.00	52.83	8
N	GLU	A	9	27.909	0.911	-7.112	1.00	54.36	7
CA	GLU	A	9	28.436	1.005	-8.474	1.00	55.52	6
CB	GLU	A	9	28.912	-0.344	-8.989	1.00	60.57	6
C	GLU	A	9	30.077	-0.937	-8.213	1.00	66.39	6
C	GLU	A	9	31.198	-1.433	-9.104	1.00	70.22	6
O	GLU	A	9	30.912	-2.114	-10.113	1.00	71.43	8
O	GLU	A	9	32.375	-1.147	-8.797	1.00	72.65	8
C	GLU	A	9	27.323	1.595	-9.339	1.00	54.98	6
O	GLU	A	9	26.219	1.047	-9.355	1.00	54.62	8
N	ILE	A	9	27.578	2.756	-9.933	1.00	54.70	7
CA	ILE	A	9	26.552	3.400	-10.753	1.00	54.44	6
CB	ILE	A	9	26.540	4.926	-10.595	1.00	53.38	6
C	ILE	A	9	25.665	5.601	-11.642	1.00	52.58	6
C	ILE	A	9	26.039	5.304	-9.195	1.00	53.52	6
C	ILE	A	9	27.133	5.719	-8.239	1.00	53.86	6
C	ILE	A	9	26.728	2.992	-12.212	1.00	54.48	6
O	ILE	A	9	27.718	3.308	-12.864	1.00	53.82	8
N	THR	A	9	25.758	2.226	-12.698	1.00	55.02	7
CA	THR	A	9	25.753	1.743	-14.070	1.00	56.18	6
CB	THR	A	9	25.556	0.214	-14.128	1.00	53.64	6
O	THR	A	9	24.276	-0.107	-13.563	1.00	51.69	8
C	THR	A	9	26.639	-0.524	-13.365	1.00	51.89	6
C	THR	A	9	24.612	2.378	-14.854	1.00	57.86	6
O	THR	A	9	23.657	2.897	-14.274	1.00	57.93	8
N	GLU	A	9	24.672	2.301	-16.180	1.00	59.43	7
CA	GLU	A	9	23.635	2.847	-17.050	1.00	60.73	6
CB	GLU	A	9	23.989	2.595	-18.517	1.00	64.29	6
C	GLU	A	9	22.926	3.011	-19.515	1.00	67.99	6

C	GLU	A	9	23.353	4.138	-20.431	1.00	70.30	6
O	GLU	A	9	22.552	5.077	-20.630	1.00	70.81	8
O	GLU	A	9	24.484	4.092	-20.959	1.00	72.24	8
C	GLU	A	9	22.261	2.275	-16.722	1.00	60.55	6
O	GLU	A	9	21.246	2.969	-16.829	1.00	60.93	8
N	GLU	A	9	22.187	1.025	-16.283	1.00	60.08	7
CA	GLU	A	9	20.972	0.362	-15.864	1.00	59.62	6
CB	GLU	A	9	21.143	-1.161	-15.975	1.00	65.14	6
C	GLU	A	9	20.576	-1.748	-17.254	1.00	70.30	6
C	GLU	A	9	21.426	-2.860	-17.834	1.00	73.39	6
O	GLU	A	9	21.214	-4.032	-17.458	1.00	74.84	8
O	GLU	A	9	22.302	-2.564	-18.674	1.00	74.99	8
C	GLU	A	9	20.570	0.709	-14.432	1.00	57.78	6
O	GLU	A	9	19.505	0.300	-13.964	1.00	58.25	8
N	ASN	A	9	21.403	1.442	-13.708	1.00	55.25	7
CA	ASN	A	9	21.154	1.857	-12.345	1.00	52.48	6
CB	ASN	A	9	22.436	1.692	-11.509	1.00	52.33	6
C	ASN	A	9	22.256	0.836	-10.279	1.00	52.34	6
O	ASN	A	9	21.147	0.414	-9.952	1.00	53.95	8
N	ASN	A	9	23.355	0.564	-9.584	1.00	52.48	7
C	ASN	A	9	20.747	3.320	-12.209	1.00	50.29	6
O	ASN	A	9	19.918	3.684	-11.376	1.00	49.91	8
N	ALA	A	9	21.390	4.190	-12.974	1.00	48.07	7
CA	ALA	A	9	21.232	5.632	-12.898	1.00	46.01	6
CB	ALA	A	9	21.670	6.263	-14.219	1.00	45.08	6
C	ALA	A	9	19.837	6.108	-12.535	1.00	44.36	6
O	ALA	A	9	19.606	6.801	-11.545	1.00	43.66	8
N	THR	A	9	18.847	5.727	-13.317	1.00	42.87	7
CA	THR	A	9	17.439	6.032	-13.183	1.00	41.55	6
CB	THR	A	9	16.725	5.210	-14.293	1.00	41.55	6
O	THR	A	9	16.719	6.004	-15.494	1.00	40.58	8
C	THR	A	9	15.307	4.783	-13.985	1.00	41.61	6
C	THR	A	9	16.812	5.788	-11.826	1.00	40.49	6
O	THR	A	9	15.785	6.415	-11.520	1.00	40.45	8
N	ARG	A	9	17.337	4.908	-10.983	1.00	39.59	7
CA	ARG	A	9	16.774	4.614	-9.680	1.00	38.37	6
CB	ARG	A	9	16.709	3.094	-9.462	1.00	38.52	6
C	ARG	A	9	15.974	2.321	-10.544	1.00	37.03	6
C	ARG	A	9	14.479	2.597	-10.499	1.00	37.03	6
N	ARG	A	9	13.865	2.041	-9.300	1.00	38.20	7
CZ	ARG	A	9	12.707	2.430	-8.785	1.00	38.63	6
N	ARG	A	9	12.002	3.397	-9.357	1.00	38.37	7
N	ARG	A	9	12.248	1.845	-7.686	1.00	38.97	7
C	ARG	A	9	17.523	5.238	-8.512	1.00	37.78	6
O	ARG	A	9	17.180	4.972	-7.356	1.00	38.19	8
N	ILE	A	1	18.586	5.988	-8.777	1.00	37.13	7
CA	ILE	A	1	19.341	6.642	-7.716	1.00	36.46	6
CB	ILE	A	1	20.835	6.276	-7.700	1.00	38.03	6
C	ILE	A	1	21.468	6.737	-6.389	1.00	36.28	6
C	ILE	A	1	21.072	4.776	-7.890	1.00	37.64	6
C	ILE	A	1	22.387	4.447	-8.564	1.00	38.13	6
C	ILE	A	1	19.222	8.160	-7.839	1.00	35.71	6
O	ILE	A	1	19.502	8.713	-8.904	1.00	35.52	8
N	GLY	A	1	18.822	8.819	-6.756	1.00	34.95	7
CA	GLY	A	1	18.705	10.273	-6.771	1.00	34.19	6
C	GLY	A	1	19.233	10.914	-5.493	1.00	33.40	6
O	GLY	A	1	20.044	10.319	-4.781	1.00	34.11	8
N	ALA	A	1	18.740	12.115	-5.193	1.00	31.57	7
CA	ALA	A	1	19.184	12.858	-4.025	1.00	29.34	6
CB	ALA	A	1	20.373	13.728	-4.437	1.00	30.70	6
C	ALA	A	1	18.123	13.747	-3.390	1.00	28.20	6
O	ALA	A	1	17.177	14.224	-4.008	1.00	28.29	8
N	ALA	A	1	18.293	13.983	-2.093	1.00	26.43	7
CA	ALA	A	1	17.403	14.814	-1.294	1.00	23.90	6

Figure 1 - 6

CB	ALA	A	1	16.330	13.994	-0.604	1.00	20.94	6
C	ALA	A	1	18.266	15.578	-0.290	1.00	23.06	6
O	ALA	A	1	18.438	15.176	0.858	1.00	22.58	8
N	ILE	A	1	18.951	16.600	-0.799	1.00	22.65	7
CA	ILE	A	1	19.890	17.384	-0.008	1.00	22.42	6
CB	ILE	A	1	21.308	17.961	-0.609	1.00	19.84	6
C	ILE	A	1	22.263	18.211	0.218	1.00	19.61	6
C	ILE	A	1	21.846	15.931	-0.727	1.00	19.04	6
C	ILE	A	1	22.912	15.769	-1.789	1.00	14.64	6
C	ILE	A	1	19.430	18.837	0.103	1.00	22.33	6
O	ILE	A	1	19.185	19.485	-0.912	1.00	22.91	8
N	GLY	A	1	19.398	19.363	1.321	1.00	21.49	7
CA	GLY	A	1	18.983	20.732	1.546	1.00	21.32	6
C	GLY	A	1	19.985	21.571	2.326	1.00	21.77	6
O	GLY	A	1	21.116	21.201	2.619	1.00	20.74	8
N	SER	A	1	19.526	22.767	2.663	1.00	22.27	7
CA	SER	A	1	20.263	23.779	3.400	1.00	22.50	6
CB	SER	A	1	21.306	24.448	2.511	1.00	22.72	6
O	SER	A	1	22.078	25.395	3.224	1.00	21.91	8
C	SER	A	1	19.248	24.811	3.895	1.00	22.77	6
O	SER	A	1	18.261	25.058	3.198	1.00	22.73	8
N	GLY	A	1	19.473	25.393	5.062	1.00	22.84	7
CA	GLY	A	1	18.557	26.368	5.619	1.00	23.14	6
C	GLY	A	1	18.683	27.762	5.036	1.00	23.90	6
O	GLY	A	1	17.665	28.437	4.846	1.00	23.26	8
N	ILE	A	1	19.904	28.234	4.800	1.00	24.27	7
CA	ILE	A	1	20.130	29.582	4.284	1.00	25.21	6
CB	ILE	A	1	20.904	30.424	5.317	1.00	28.84	6
C	ILE	A	1	21.399	31.746	4.750	1.00	29.40	6
C	ILE	A	1	20.025	30.718	6.544	1.00	30.94	6
C	ILE	A	1	20.804	31.053	7.796	1.00	32.04	6
C	ILE	A	1	20.839	29.580	2.938	1.00	25.28	6
O	ILE	A	1	20.712	30.527	2.153	1.00	25.17	8
N	GLY	A	1	21.587	28.527	2.623	1.00	25.28	7
CA	GLY	A	1	22.284	28.453	1.345	1.00	25.24	6
C	GLY	A	1	23.457	29.418	1.274	1.00	25.63	6
O	GLY	A	1	24.083	29.755	2.279	1.00	25.92	8
N	GLY	A	1	23.862	29.789	0.062	1.00	25.45	7
CA	GLY	A	1	25.084	30.496	-0.218	1.00	26.20	6
C	GLY	A	1	25.213	31.934	0.223	1.00	27.33	6
O	GLY	A	1	25.522	32.817	-0.585	1.00	27.71	8
N	LEU	A	1	25.181	32.186	1.526	1.00	27.58	7
CA	LEU	A	1	25.252	33.513	2.104	1.00	26.89	6
CB	LEU	A	1	25.045	33.438	3.622	1.00	30.54	6
C	LEU	A	1	23.844	34.161	4.225	1.00	33.04	6
C	LEU	A	1	23.965	34.212	5.744	1.00	34.23	6
C	LEU	A	1	23.678	35.565	3.670	1.00	31.51	6
C	LEU	A	1	26.579	34.203	1.822	1.00	25.55	6
O	LEU	A	1	26.623	35.387	1.493	1.00	24.44</	

C	ILE	A	1	23.320	37.452	-1.351	1.00	20.68	6
C	ILE	A	1	23.558	35.053	-2.019	1.00	21.17	6
C	ILE	A	1	22.467	34.395	-1.206	1.00	20.81	6
C	ILE	A	1	26.148	37.861	-1.461	1.00	22.38	6
O	ILE	A	1	25.969	38.896	-2.103	1.00	21.79	8
N	GLU	A	1	26.848	37.829	-0.332	1.00	22.40	7
CA	GLU	A	1	27.490	39.019	0.209	1.00	23.90	6
CB	GLU	A	1	28.076	38.737	1.590	1.00	23.43	6
C	GLU	A	1	27.029	38.487	2.666	1.00	24.28	6
C	GLU	A	1	27.682	38.221	4.010	1.00	26.12	6
O	GLU	A	1	27.217	37.322	4.736	1.00	24.90	8
O	GLU	A	1	28.671	38.918	4.318	1.00	28.72	8
C	GLU	A	1	28.575	39.538	-0.727	1.00	24.96	6
O	GLU	A	1	28.586	40.724	-1.050	1.00	25.66	8
N	GLU	A	1	29.464	38.665	-1.189	1.00	26.22	7
CA	GLU	A	1	30.525	39.052	-2.107	1.00	27.40	6
CB	GLU	A	1	31.361	37.838	-2.520	1.00	29.69	6
C	GLU	A	1	32.500	38.186	-3.466	1.00	36.82	6
C	GLU	A	1	33.298	36.974	-3.901	1.00	39.85	6
O	GLU	A	1	34.033	36.420	-3.058	1.00	42.55	8
O	GLU	A	1	33.191	36.575	-5.079	1.00	43.21	8
C	GLU	A	1	29.968	39.727	-3.358	1.00	27.74	6
O	GLU	A	1	30.345	40.847	-3.698	1.00	27.49	8
N	ASN	A	1	29.038	39.051	-4.026	1.00	27.54	7
CA	ASN	A	1	28.397	39.569	-5.223	1.00	27.47	6
CB	ASN	A	1	27.450	38.524	-5.823	1.00	25.94	6
C	ASN	A	1	28.191	37.404	-6.525	1.00	24.69	6
O	ASN	A	1	28.773	37.602	-7.591	1.00	25.98	8
N	ASN	A	1	28.168	36.214	-5.940	1.00	22.87	7
C	ASN	A	1	27.639	40.862	-4.958	1.00	27.92	6
O	ASN	A	1	27.674	41.763	-5.801	1.00	27.84	8
N	HIS	A	1	26.965	40.976	-3.811	1.00	28.73	7
CA	HIS	A	1	26.266	42.219	-3.503	1.00	29.88	6
CB	HIS	A	1	25.334	42.129	-2.295	1.00	26.18	6
C	HIS	A	1	24.463	43.353	-2.216	1.00	23.31	6
C	HIS	A	1	24.431	44.382	-1.343	1.00	22.00	6
N	HIS	A	1	23.484	43.614	-3.151	1.00	23.32	7
CE	HIS	A	1	22.881	44.750	-2.852	1.00	23.34	6
N	HIS	A	1	23.438	45.235	-1.755	1.00	23.46	7
C	HIS	A	1	27.290	43.339	-3.321	1.00	31.26	6
O	HIS	A	1	27.141	44.417	-3.898	1.00	31.42	8
N	THR	A	1	28.382	43.048	-2.620	1.00	32.61	7
CA	THR	A	1	29.466	44.011	-2.448	1.00	33.99	6
CB	THR	A	1	30.580	43.428	-1.562	1.00	34.40	6
O	THR	A	1	30.011	43.087	-0.288	1.00	33.02	8
C	THR	A	1	31.707	44.425	-1.345	1.00	35.33	6
C	THR	A	1	30.018	44.464	-3.792	1.00	34.89	6
O	THR	A	1	30.148	45.668	-4.033	1.00	35.35	8
N	SER	A	1	30.289	43.527	-4.695	1.00	35.14	7
CA	SER	A	1	30.726	43.862	-6.047	1.00	35.99	6
CB	SER	A	1	30.916	42.588	-6.870	1.00	35.21	6
O	SER	A	1	31.858	41.733	-6.236	1.00	37.30	8
C	SER	A	1	29.734	44.807	-6.711	1.00	37.29	6
O	SER	A	1	30.092	45.918	-7.100	1.00	37.19	8
N	LEU	A	1	28.464	44.426	-6.777	1.00	38.61	7
CA	LEU	A	1	27.411	45.250	-7.350	1.00	40.26	6
CB	LEU	A	1	26.054	44.565	-7.172	1.00	39.02	6
C	LEU	A	1	24.786	45.386	-7.405	1.00	37.46	6
C	LEU	A	1	24.538	45.621	-8.887	1.00	35.37	6
C	LEU	A	1	23.583	44.700	-6.770	1.00	34.67	6
C	LEU	A	1	27.377	46.657	-6.775	1.00	42.20	6
O	LEU	A	1	27.267	47.624	-7.535	1.00	42.75	8
N	MET	A	1	27.473	46.815	-5.461	1.00	44.22	7
CA	MET	A	1	27.448	48.194	-4.896	1.00	46.59	6

Figure 1 - 7

CA	VAL	A	1	19.895	25.653	-2.121	1.00	25.35	6
CB	VAL	A	1	18.603	25.780	-1.273	1.00	27.33	6
C	VAL	A	1	18.095	24.469	-0.709	1.00	29.41	6
C	VAL	A	1	18.866	26.764	-0.133	1.00	28.85	6
C	VAL	A	1	19.959	24.312	-2.815	1.00	25.00	6
O	VAL	A	1	20.571	23.385	-2.257	1.00	24.69	8
N	ASN	A	1	19.368	24.140	-3.991	1.00	24.21	7
CA	ASN	A	1	19.357	22.841	-4.651	1.00	24.07	6
CB	ASN	A	1	18.105	22.748	-5.540	1.00	22.14	6
C	ASN	A	1	18.226	23.637	-6.762	1.00	22.88	6
O	ASN	A	1	18.291	24.859	-6.633	1.00	22.25	8
N	ASN	A	1	18.316	23.019	-7.933	1.00	22.17	7
C	ASN	A	1	20.613	22.517	-5.443	1.00	24.43	6
O	ASN	A	1	20.701	21.419	-6.008	1.00	23.79	8
N	MET	A	1	21.630	23.371	-5.435	1.00	25.03	7
CA	MET	A	1	22.850	23.139	-6.196	1.00	26.58	6
CB	MET	A	1	23.547	24.458	-6.529	1.00	27.98	6
C	MET	A	1	22.821	25.227	-7.629	1.00	32.05	6
SD	MET	A	1	22.346	24.205	-9.040	1.00	35.93	1
CE	MET	A	1	23.951	23.688	-9.643	1.00	36.90	6
C	MET	A	1	23.777	22.099	-5.593	1.00	27.33	6
O	MET	A	1	24.655	21.602	-6.317	1.00	28.18	8
N	VAL	A	1	23.598	21.699	-4.337	1.00	27.13	7
CA	VAL	A	1	24.425	20.637	-3.771	1.00	27.35	6
CB	VAL	A	1	24.341	20.475	-2.251	1.00	27.90	6
C	VAL	A	1	25.268	19.352	-1.785	1.00	25.87	6
C	VAL	A	1	24.698	21.767	-1.536	1.00	25.87	6
C	VAL	A	1	23.973	19.328	-4.435	1.00	27.41	6
O	VAL	A	1	24.783	18.507	-4.856	1.00	28.08	8
N	ALA	A	1	22.658	19.158	-4.561	1.00	27.02	7
CA	ALA	A	1	22.079	17.988	-5.214	1.00	26.49	6
CB	ALA	A	1	20.598	17.856	-4.897	1.00	21.24	6
C	ALA	A	1	22.302	18.059	-6.723	1.00	26.51	6
O	ALA	A	1	22.549	17.048	-7.378	1.00	25.54	8
N	GLY	A	1	22.291	19.270	-7.275	1.00	27.35	7
CA	GLY	A	1	22.623	19.479	-8.678	1.00	28.51	6
C	GLY	A	1	24.041	18.991	-8.970	1.00	29.26	6
O	GLY	A	1	24.238	18.218	-9.905	1.00	29.73	8
N	HIS	A	1	25.018	19.404	-8.172	1.00	30.44	7
CA	HIS	A	1	26.403	19.012	-8.362	1.00	31.50	6
CB	HIS	A	1	27.347	19.828	-7.458	1.00	31.18	6
C	HIS	A	1	27.723	21.121	-8.124	1.00	30.77	6
C	HIS	A	1	28.449	21.359	-9.242	1.00	29.89	6
N	HIS	A	1	27.298	22.347	-7.668	1.00	31.84	7
CE	HIS	A	1	27.765	23.293	-8.467	1.00	31.24	6
N	HIS	A	1	28.464	22.719	-9.430	1.00	28.66	7
C	HIS	A	1	26.666	17.528	-8.173	1.00	32.17	6
O	HIS	A	1	27.415	16.950	-8.967	1.00	31.93	8
N	LEU	A	1	26.070	16.905	-7.163	1.00	33.38	7
CA	LEU	A	1	26.284	15.480	-6.932	1.00	34.08	6
CB	LEU	A	1	25.766	15.068	-5.555	1.00	33.94	6
C	LEU	A	1	26.696	15.347	-4.370	1.00	35.38	6
C	LEU	A	1	26.024	14.968	-3.059	1.00	33.09	6
C	LEU	A	1	28.019	14.607	-4.510	1.00	35.02	6
C	LEU	A	1	25.667	14.626	-8.032	1.00	34.56	6
O	LEU	A	1	26.298	13.669	-8.492	1.00	34.56	8
N	THR	A	1	24.459	14.963	-8.475	1.00	34.57	7
CA	THR	A	1	23.785	14.223	-9.532	1.00	34.15	6
CB	THR	A	1	22.420	14.826	-9.914	1.00	29.47	6
O	THR	A	1	22.582	16.220	-10.197	1.00	26.25	8
C	THR	A	1	21.395	14.651	-8.809	1.00	24.88	6
C	THR	A	1	24.646	14.159	-10.792	1.00	35.65	6
O	THR	A	1	24.850	13.081	-11.350	1.00	35.92	8
N	ILE	A	1	25.147	15.306	-11.241	1.00	36.68	7

CA	ILE	A	1	26.035	15.369	-12.394	1.00	37.59	6
CB	ILE	A	1	26.478	16.811	-12.704	1.00	38.89	6
C	ILE	A	1	27.394	16.854	-13.919	1.00	37.93	6
C	ILE	A	1	25.266	17.723	-12.924	1.00	38.70	6
C	ILE	A	1	25.565	19.186	-12.670	1.00	37.99	6
C	ILE	A	1	27.283	14.521	-12.164	1.00	37.96	6
O	ILE	A	1	27.627	13.656	-12.966	1.00	38.29	8
N	MET	A	1	27.967	14.762	-11.053	1.00	37.90	7
CA	MET	A	1	29.175	14.047	-10.686	1.00	38.24	6
CB	MET	A	1	29.616	14.468	-9.277	1.00	39.44	6
C	MET	A	1	30.324	15.813	-9.239	1.00	40.87	6
SD	MET	A	1	30.886	16.247	-7.581	1.00	42.12	1
CE	MET	A	1	32.332	15.198	-7.440	1.00	41.22	6
C	MET	A	1	29.056	12.531	-10.747	1.00	37.94	6
O	MET	A	1	29.979	11.880	-11.247	1.00	38.17	8
N	TYR	A	1	27.984	11.945	-10.223	1.00	37.10	7
CA	TYR	A	1	27.818	10.501	-10.220	1.00	36.19	6
CB	TYR	A	1	27.350	10.040	-8.822	1.00	36.32	6
C	TYR	A	1	28.508	10.115	-7.843	1.00	36.68	6
C	TYR	A	1	28.715	11.251	-7.073	1.00	36.50	6
CE	TYR	A	1	29.778	11.325	-6.193	1.00	36.74	6
C	TYR	A	1	29.399	9.058	-7.720	1.00	36.65	6
CE	TYR	A	1	30.463	9.127	-6.840	1.00	36.77	6
CZ	TYR	A	1	30.647	10.262	-6.080	1.00	36.77	6
O	TYR	A	1	31.705	10.334	-5.205	1.00	37.18	8
C	TYR	A	1	26.857	9.974	-11.272	1.00	35.61	6
O	TYR	A	1	26.628	8.761	-11.334	1.00	35.78	8
N	GLY	A	1	26.245	10.850	-12.060	1.00	34.65	7
CA	GLY	A	1	25.277	10.432	-13.063	1.00	33.62	6
C	GLY	A	1	23.987	9.912	-12.443	1.00	33.64	6
O	GLY	A	1	23.404	8.949	-12.947	1.00	32.91	8
N	LEU	A	1	23.524	10.551	-11.371	1.00	33.89	7
CA	LEU	A	1	22.277	10.155	-10.718	1.00	34.12	6
CB	LEU	A	1	22.255	10.578	-9.253	1.00	34.78	6
C	LEU	A	1	23.480	10.255	-8.399	1.00	36.43	6
C	LEU	A	1	23.386	10.932	-7.038	1.00	36.23	6
C	LEU	A	1	23.656	8.753	-8.225	1.00	36.82	6
C	LEU	A	1	21.095	10.757	-11.474	1.00	34.20	6
O	LEU	A	1	20.954	11.976	-11.573	1.00	34.71	8
N	ARG	A	1	20.275	9.896	-12.067	1.00	34.03	7
CA	ARG	A	1	19.162	10.333	-12.899	1.00	33.73	6
CB	ARG	A	1	19.212	9.617	-14.255	1.00	37.33	6
C	ARG	A	1	20.590	9.564	-14.892	1.00	39.93	6
C	ARG	A	1	20.559	9.681	-16.405	1.00	45.40	6
N	ARG	A	1	19.555	8.819	-17.010	1.00	50.00	7
CZ	ARG	A	1	18.668	9.187	-17.925	1.00	52.17	6
N	ARG	A	1	18.637	10.432	-18.380	1.00	53.86	7
N	ARG	A	1	17.795	8.302	-18.391	1.00	53.95	7
C	ARG	A	1	17.811	10.130	-12.228	1.00	32.95	6
O	ARG	A	1	16.766	10.388	-12.826	1.00	32.75	8
N	GLY	A	1	17.824	9.688	-10.975	1.00	32.29	7
CA	GLY	A	1	16.593	9.481	-10.221	1.00	31.31	6
C	GLY	A	1	16.101	10.809	-9.649	1.00	30.98	6
O	GLY	A	1	16.608	11.880	-9.981	1.00	30.61	8
N	PRO	A	1	15.096	10.737	-8.780	1.00	30.29	7
C	PRO	A	1	14.456	9.478	-8.332	1.00	30.09	6
CA	PRO	A	1	14.509	11.909	-8.166	1.00	29.57	6
CB	PRO	A	1	13.519	11.360	-7.154	1.00	29.77	6
C	PRO	A	1	13.355	9.915	-7.418	1.00	29.79	6
C	PRO	A	1	15.533	12.807	-7.488	1.00	29.38	6
O	PRO	A	1	16.450	12.336	-6.817	1.00	28.41	8
N	SER	A	1	15.356	14.118	-7.629	1.00	28.94	7
CA	SER	A	1	16.250	15.094	-7.023	1.00	27.53	6
CB	SER	A	1	17.149	15.708	-8.103	1.00	29.57	6

Figure 1 - 9

O	SER	A	1	18.098	16.586	-7.525	1.00	33.35	8
C	SER	A	1	15.482	16.210	-6.329	1.00	26.68	6
O	SER	A	1	14.883	17.041	-7.016	1.00	26.03	8
N	ILE	A	1	15.474	16.244	-4.995	1.00	26.03	7
CA	ILE	A	1	14.787	17.320	-4.297	1.00	25.17	6
CB	ILE	A	1	13.482	16.951	-3.579	1.00	24.96	6
C	ILE	A	1	12.331	16.776	-4.559	1.00	22.35	6
C	ILE	A	1	13.650	15.714	-2.691	1.00	22.54	6
C	ILE	A	1	12.588	15.627	-1.610	1.00	19.83	6
C	ILE	A	1	15.709	17.968	-3.259	1.00	25.23	6
O	ILE	A	1	16.762	17.455	-2.899	1.00	24.97	8
N	SER	A	1	15.272	19.131	-2.791	1.00	23.95	7
CA	SER	A	1	15.975	19.891	-1.776	1.00	23.50	6
CB	SER	A	1	16.846	20.992	-2.374	1.00	22.64	6
O	SER	A	1	17.886	20.488	-3.183	1.00	24.55	8
C	SER	A	1	14.954	20.529	-0.830	1.00	22.76	6
O	SER	A	1	14.208	21.410	-1.268	1.00	22.27	8
N	ILE	A	1	14.925	20.083	0.422	1.00	21.99	7
CA	ILE	A	1	13.988	20.677	1.379	1.00	21.74	6
CB	ILE	A	1	13.273	19.657	2.271	1.00	19.43	6
C	ILE	A	1	12.340	20.363	3.253	1.00	18.21	6
C	ILE	A	1	12.485	18.680	1.394	1.00	16.47	6
C	ILE	A	1	11.801	17.553	2.125	1.00	15.87	6
C	ILE	A	1	14.732	21.721	2.212	1.00	21.86	6
O	ILE	A	1	15.832	21.490	2.710	1.00	22.41	8
N	ALA	A	1	14.136	22.904	2.305	1.00	21.42	7
CA	ALA	A	1	14.730	24.012	3.047	1.00	20.33	6
CB	ALA	A	1	15.008	25.172	2.105	1.00	16.53	6
C	ALA	A	1	13.798	24.428	4.180	1.00	19.82	6
O	ALA	A	1	12.924	25.278	4.015	1.00	18.81	8
N	THR	A	1	13.981	23.797	5.336	1.00	19.95	7
CA	THR	A	1	13.149	24.098	6.499	1.00	20.29	6
CB	THR	A	1	12.256	22.902	6.879	1.00	18.29	6
O	THR	A	1	13.009	21.692	6.725	1.00	17.31	8
C	THR	A	1	11.023	22.835	5.992	1.00	13.32	6
C	THR	A	1	14.011	24.514	7.684	1.00	20.40	6
O	THR	A	1	13.897	23.945	8.770	1.00	20.37	8
N	ALA	A	1	14.905	25.476	7.453	1.00	20.45	7
CA	ALA	A	1	15.764	25.976	8.530	1.00	21.02	6
CB	ALA	A	1	14.946	26.878	9.445	1.00	18.59	6
C	ALA	A	1	16.387	24.821	9.297	1.00	21.40	6
O	ALA	A	1	16.920	23.888	8.690	1.00	21.38	8
N	CYS	A	1	16.226	24.780	10.615	1.00	22.02	7
CA	CYS	A	1	16.747	23.748	11.482	1.00	22.36	6
CB	CYS	A	1	16.442	24.074	12.957	1.00	21.11	6
SG	CYS	A	1	16.391	25.832	13.348	1.00	19.89	1
C	CYS	A	1	16.234	22.335	11.252	1.00	23.18	6
O	CYS	A	1	16.802	21.406	11.841	1.00	24.80	8
N	THR	A	1	15.163	22.137	10.504	1.00	23.36	7
CA									

O	GLY	A	1	17.502	15.461	7.132	1.00	24.80	8
N	VAL	A	1	16.529	16.677	8.744	1.00	25.23	7
CA	VAL	A	1	15.568	15.639	9.104	1.00	26.31	6
CB	VAL	A	1	14.954	15.935	10.485	1.00	26.54	6
C	VAL	A	1	13.631	15.222	10.713	1.00	28.08	6
C	VAL	A	1	15.946	15.553	11.579	1.00	25.33	6
C	VAL	A	1	14.485	15.475	8.048	1.00	26.62	6
O	VAL	A	1	14.045	14.351	7.792	1.00	27.98	8
N	HIS	A	1	14.039	16.570	7.442	1.00	26.00	7
CA	HIS	A	1	12.999	16.512	6.424	1.00	24.82	6
CB	HIS	A	1	12.453	17.908	6.120	1.00	23.96	6
C	HIS	A	1	11.405	18.394	7.069	1.00	23.62	6
C	HIS	A	1	10.606	17.745	7.947	1.00	22.84	6
N	HIS	A	1	11.084	19.733	7.180	1.00	22.53	7
CE	HIS	A	1	10.136	19.880	8.085	1.00	21.95	6
N	HIS	A	1	9.828	18.691	8.571	1.00	22.11	7
C	HIS	A	1	13.505	15.866	5.138	1.00	24.05	6
O	HIS	A	1	12.780	15.110	4.489	1.00	23.48	8
N	ASN	A	1	14.738	16.191	4.760	1.00	23.02	7
CA	ASN	A	1	15.337	15.637	3.551	1.00	22.46	6
CB	ASN	A	1	16.657	16.341	3.249	1.00	20.13	6
C	ASN	A	1	16.509	17.666	2.535	1.00	19.01	6
O	ASN	A	1	16.753	18.736	3.102	1.00	20.03	8
N	ASN	A	1	16.117	17.630	1.268	1.00	14.76	7
C	ASN	A	1	15.532	14.131	3.684	1.00	22.99	6
O	ASN	A	1	15.091	13.358	2.832	1.00	23.06	8
N	ILE	A	1	16.123	13.691	4.791	1.00	23.65	7
CA	ILE	A	1	16.336	12.273	5.057	1.00	24.37	6
CB	ILE	A	1	17.089	12.047	6.382	1.00	23.70	6
C	ILE	A	1	17.092	10.579	6.787	1.00	22.39	6
C	ILE	A	1	18.523	12.568	6.258	1.00	22.09	6
C	ILE	A	1	19.263	12.683	7.570	1.00	23.14	6
C	ILE	A	1	15.023	11.497	5.061	1.00	24.26	6
O	ILE	A	1	14.932	10.445	4.427	1.00	23.49	8
N	GLY	A	1	14.012	11.997	5.762	1.00	24.58	7
CA	GLY	A	1	12.713	11.349	5.812	1.00	25.44	6
C	GLY	A	1	11.980	11.315	4.479	1.00	25.99	6
O	GLY	A	1	11.320	10.312	4.179	1.00	26.63	8
N	HIS	A	1	12.080	12.365	3.659	1.00	25.24	7
CA	HIS	A	1	11.370	12.367	2.374	1.00	25.23	6
CB	HIS	A	1	10.991	13.778	1.924	1.00	22.39	6
C	HIS	A	1	9.705	14.164	2.612	1.00	19.50	6
C	HIS	A	1	8.432	13.773	2.381	1.00	18.58	6
N	HIS	A	1	9.662	14.997	3.705	1.00	19.92	7
CE	HIS	A	1	8.411	15.125	4.108	1.00	18.51	6
N	HIS	A	1	7.645	14.391	3.321	1.00	18.63	7
C	HIS	A	1	12.110	11.526	1.352	1.00	25.82	6
O	HIS	A	1	11.508	10.936	0.451	1.00	25.77	8
N	ALA	A	1	13.415	11.347	1.551	1.00	26.62	7
CA	ALA	A	1	14.201	10.450	0.711	1.00	27.35	6
CB	ALA	A	1	15.678	10.562	1.039	1.00	27.03	6
C	ALA	A	1	13.708	9.019	0.957	1.00	27.92	6
O	ALA	A	1	13.531	8.234	0.027	1.00	28.61	8
N	ALA	A	1	13.412	8.701	2.216	1.00	27.72	7
CA	ALA	A	1	12.864	7.411	2.605	1.00	28.34	6
CB	ALA	A	1	12.932	7.219	4.111	1.00	24.59	6
C	ALA	A	1	11.434	7.241	2.103	1.00	28.66	6
O	ALA	A	1	11.083	6.159	1.626	1.00	29.30	8
N	ARG	A	1	10.626	8.298	2.173	1.00	28.76	7
CA	ARG	A	1	9.262	8.225	1.648	1.00	28.61	6
CB	ARG	A	1	8.456	9.488	1.913	1.00	24.10	6
C	ARG	A	1	8.154	9.789	3.365	1.00	23.11	6
C	ARG	A	1	7.081	8.881	3.938	1.00	24.33	6
N	ARG	A	1	6.449	9.447	5.126	1.00	24.09	7

Figure 1 - 10

CA	VAL	A	1	18.917	4.578	-3.508	1.00	33.83	6
CB	VAL	A	1	20.345	4.287	-4.011	1.00	35.53	6
C	VAL	A	1	21.388	4.950	-3.114	1.00	36.35	6
C	VAL	A	1	20.639	2.798	-4.108	1.00	35.37	6
C	VAL	A	1	18.733	6.096	-3.518	1.00	33.19	6
O	VAL	A	1	18.432	6.683	-4.555	1.00	33.44	8
N	MET	A	1	18.951	6.739	-2.378	1.00	32.55	7
CA	MET	A	1	18.937	8.186	-2.263	1.00	31.13	6
CB	MET	A	1	17.660	8.727	-1.631	1.00	29.51	6
C	MET	A	1	16.342	8.551	-2.341	1.00	29.70	6
SD	MET	A	1	16.246	9.357	-3.946	1.00	29.08	1
CE	MET	A	1	15.597	10.961	-3.486	1.00	31.20	6
C	MET	A	1	20.109	8.666	-1.395	1.00	30.44	6
O	MET	A	1	20.302	8.170	-0.284	1.00	29.87	8
N	VAL	A	1	20.857	9.642	-1.890	1.00	29.52	7
CA	VAL	A	1	21.815	10.382	-1.073	1.00	28.81	6
CB	VAL	A	1	22.956	11.026	-1.865	1.00	30.53	6
C	VAL	A	1	24.149	11.320	-0.962	1.00	29.68	6
C	VAL	A	1	23.391	10.162	-3.041	1.00	32.18	6
C	VAL	A	1	21.003	11.492	-0.394	1.00	28.25	6
O	VAL	A	1	20.334	12.247	-1.103	1.00	28.36	8
N	ALA	A	1	21.009	11.563	0.927	1.00	28.00	7
CA	ALA	A	1	20.229	12.580	1.623	1.00	27.92	6
CB	ALA	A	1	19.000	11.963	2.275	1.00	24.93	6
C	ALA	A	1	21.058	13.294	2.684	1.00	28.72	6
O	ALA	A	1	22.054	12.756	3.172	1.00	30.05	8
N	GLY	A	1	20.628	14.502	3.037	1.00	27.99	7
CA	GLY	A	1	21.336	15.263	4.055	1.00	27.29	6
C	GLY	A	1	21.168	16.765	3.879	1.00	26.54	6
O	GLY	A	1	20.284	17.256	3.181	1.00	26.98	8
N	GLY	A	1	22.058	17.494	4.543	1.00	25.00	7
CA	GLY	A	1	22.044	18.947	4.497	1.00	23.84	6
C	GLY	A	1	23.474	19.468	4.611	1.00	23.62	6
O	GLY	A	1	24.391	18.762	5.026	1.00	23.67	8
N	ALA	A	1	23.636	20.717	4.211	1.00	22.65	7
CA	ALA	A	1	24.920	21.397	4.285	1.00	22.01	6
CB	ALA	A	1	25.707	21.264	3.001	1.00	20.15	6
C	ALA	A	1	24.631	22.862	4.618	1.00	21.60	6
O	ALA	A	1	23.618	23.403	4.182	1.00	21.84	8
N	GLU	A	1	25.487	23.458	5.429	1.00	20.83	7
CA	GLU	A	1	25.319	24.851	5.816	1.00	19.89	6
CB	GLU	A	1	24.426	24.977	7.049	1.00	18.28	6
C	GLU	A	1	23.831	26.355	7.291	1.00	18.28	6
C	GLU	A	1	22.489	26.516	6.598	1.00	18.67	6
O	GLU	A	1	21.572	25.707	6.865	1.00	19.58	8
O	GLU	A	1	22.362	27.441	5.773	1.00	16.71	8
C	GLU	A	1	26.686	25.469	6.094	1.00	19.29	6
O	GLU	A	1	27.621	24.801	6.521	1.00	18.97	8
N	LYS	A	1	26.786	26.757	5.833	1.00	19.94	7
CA	LYS	A	1	27.969	27.550	6.134	1.00	20.57	6
CB	LYS	A	1	29.088	27.407	5.117	1.00	23.02	6
C	LYS	A	1	30.476	27.636	5.704	1.00	21.33	6
C	LYS	A	1	30.817	29.119	5.749	1.00	20.79	6
CE	LYS	A	1	32.283	29.325	6.102	1.00	18.62	6
NZ	LYS	A	1	32.453	30.430	7.087	1.00	22.09	7
C	LYS	A	1	27.477	28.996	6.252	1.00	21.04	6
O	LYS	A	1	27.588	29.801	5.335	1.00	21.85	8
N	ALA	A	1	26.826	29.254	7.380	1.00	21.26	7
CA	ALA	A	1	26.207	30.540	7.651	1.00	22.03	6
CB	ALA	A	1	24.777	30.350	8.145	1.00	17.02	6
C	ALA	A	1	27.006	31.365	8.643	1.00	23.37	6
O	ALA	A	1	26.490	32.344	9.197	1.00	25.73	8
N	SER	A	1	28.278	31.032	8.842	1.00	23.12	7
CA	SER	A	1	29.124	31.824	9.733	1.00	23.49	6

Figure 1 - 11

CA	PHE	A	2	22.371	29.067	20.587	1.00	25.74	6
CB	PHE	A	2	21.471	28.412	19.546	1.00	25.79	6
C	PHE	A	2	21.216	29.119	18.254	1.00	24.95	6
C	PHE	A	2	22.114	29.029	17.203	1.00	24.19	6
C	PHE	A	2	20.068	29.876	18.077	1.00	23.27	6
CE	PHE	A	2	21.878	29.680	16.007	1.00	25.52	6
CE	PHE	A	2	19.825	30.531	16.884	1.00	24.37	6
CZ	PHE	A	2	20.731	30.434	15.848	1.00	25.52	6
C	PHE	A	2	23.710	29.499	20.011	1.00	23.85	6
O	PHE	A	2	24.058	30.676	19.954	1.00	22.69	8
N	VAL	A	2	24.512	28.501	19.649	1.00	23.40	7
CA	VAL	A	2	25.827	28.727	19.061	1.00	23.14	6
CB	VAL	A	2	26.963	28.060	19.845	1.00	21.81	6
C	VAL	A	2	28.308	28.317	19.177	1.00	21.07	6
C	VAL	A	2	27.009	28.565	21.282	1.00	26.15	6
C	VAL	A	2	25.815	28.227	17.615	1.00	22.86	6
O	VAL	A	2	25.369	27.121	17.331	1.00	21.50	8
N	LEU	A	2	26.245	29.082	16.701	1.00	23.86	7
CA	LEU	A	2	26.240	28.798	15.274	1.00	25.13	6
CB	LEU	A	2	26.346	30.119	14.519	1.00	29.61	6
C	LEU	A	2	25.871	30.274	13.085	1.00	33.44	6
C	LEU	A	2	24.777	29.293	12.696	1.00	35.45	6
C	LEU	A	2	25.382	31.707	12.865	1.00	34.21	6
C	LEU	A	2	27.377	27.868	14.868	1.00	25.05	6
O	LEU	A	2	28.507	28.038	15.327	1.00	25.49	8
N	GLY	A	2	27.086	26.903	14.001	1.00	24.15	7
CA	GLY	A	2	28.085	25.959	13.531	1.00	24.11	6
C	GLY	A	2	27.960	25.662	12.042	1.00	24.67	6
O	GLY	A	2	26.880	25.754	11.456	1.00	25.37	8
N	ASP	A	2	29.069	25.277	11.419	1.00	24.44	7
CA	ASP	A	2	29.110	24.945	10.007	1.00	23.88	6
CB	ASP	A	2	30.222	25.682	9.261	1.00	23.99	6
C	ASP	A	2	30.213	27.180	9.450	1.00	24.50	6
O	ASP	A	2	29.125	27.786	9.377	1.00	29.71	8
O	ASP	A	2	31.298	27.752	9.676	1.00	25.78	8
C	ASP	A	2	29.361	23.450	9.804	1.00	23.41	6
O	ASP	A	2	29.973	22.805	10.654	1.00	23.79	8
N	GLY	A	2	28.949	22.941	8.644	1.00	22.27	7
CA	GLY	A	2	29.191	21.541	8.336	1.00	21.31	6
C	GLY	A	2	28.186	20.948	7.363	1.00	20.58	6
O	GLY	A	2	27.441	21.636	6.671	1.00	20.04	8
N	ALA	A	2	28.193	19.621	7.305	1.00	20.48	7
CA	ALA	A	2	27.344	18.872	6.393	1.00	21.61	6
CB	ALA	A	2	27.762	19.108	4.948	1.00	20.78	6
C	ALA	A	2	27.433	17.380	6.706	1.00	21.99	6
O	ALA	A	2	28.522	16.846	6.890	1.00	22.37	8
N	GLY	A	2	26.278	16.745	6.779	1.00	22.26	7
CA	GLY	A	2	26.193	15.310	7.029	1.00	23.98	6
C	GLY	A	2	25.442	14.711	5.837	1.00	25.43	6
O	GLY	A	2	24.558	15.374	5.292	1.00	25.88	8
N	MET	A	2	25.809	13.502	5.442	1.00	26.56	7
CA	MET	A	2	25.162	12.884	4.284	1.00	27.91	6
CB	MET	A	2	25.987	13.213	3.041	1.00	27.89	6
C	MET	A	2	25.234	13.503	1.769	1.00	30.30	6
SD	MET	A	2	24.418	15.099	1.678	1.00	31.13	1
CE	MET	A	2	25.677	16.204	2.299	1.00	32.90	6
C	MET	A	2	25.054	11.381	4.482	1.00	29.36	6
O	MET	A	2	26.020	10.774	4.952	1.00	30.39	8
N	LEU	A	2	23.891	10.802	4.184	1.00	29.56	7
CA	LEU	A	2	23.748	9.362	4.290	1.00	30.24	6
CB	LEU	A	2	22.869	8.838	5.406	1.00	30.18	6
C	LEU	A	2	22.076	9.717	6.348	1.00	29.17	6
C	LEU	A	2	21.017	8.902	7.084	1.00	29.29	6
C	LEU	A	2	22.986	10.389	7.364	1.00	30.62	6

C	LEU	A	2	23.205	8.789	2.973	1.00	31.47	6
O	LEU	A	2	22.504	9.447	2.213	1.00	32.20	8
N	VAL	A	2	23.559	7.529	2.753	1.00	31.86	7
CA	VAL	A	2	23.031	6.776	1.629	1.00	32.03	6
CB	VAL	A	2	24.033	5.825	0.970	1.00	31.99	6
C	VAL	A	2	23.378	5.082	-0.190	1.00	33.53	6
C	VAL	A	2	25.261	6.577	0.485	1.00	31.64	6
C	VAL	A	2	21.851	5.964	2.178	1.00	32.37	6
O	VAL	A	2	22.003	5.194	3.124	1.00	32.10	8
N	LEU	A	2	20.675	6.234	1.633	1.00	32.90	7
CA	LEU	A	2	19.473	5.506	2.023	1.00	32.91	6
CB	LEU	A	2	18.307	6.453	2.270	1.00	32.52	6
C	LEU	A	2	18.303	7.271	3.561	1.00	31.91	6
C	LEU	A	2	17.139	8.254	3.566	1.00	32.20	6
C	LEU	A	2	18.230	6.865	4.779	1.00	33.24	6
C	LEU	A	2	19.146	4.547	0.882	1.00	33.63	6
O	LEU	A	2	19.229	4.984	-0.271	1.00	33.36	8
N	GLU	A	2	18.806	3.297	1.169	1.00	35.24	7
CA	GLU	A	2	18.428	2.403	0.074	1.00	37.02	6
CB	GLU	A	2	19.635	1.854	-0.663	1.00	39.18	6
C	GLU	A	2	20.444	0.775	0.026	1.00	41.57	6
C	GLU	A	2	21.610	0.335	-0.845	1.00	43.33	6
O	GLU	A	2	22.733	0.832	-0.631	1.00	42.15	8
O	GLU	A	2	21.393	-0.501	-1.748	1.00	46.02	8
C	GLU	A	2	17.490	1.295	0.538	1.00	37.80	6
O	GLU	A	2	17.315	1.048	1.729	1.00	37.74	8
N	GLU	A	2	16.774	0.747	-0.440	1.00	38.04	7
CA	GLU	A	2	15.789	-0.298	-0.182	1.00	38.80	6
CB	GLU	A	2	14.981	-0.568	-1.450	1.00	38.06	6
C	GLU	A	2	13.782	-1.481	-1.233	1.00	33.93	6
C	GLU	A	2	14.167	-2.937	-1.445	1.00	33.44	6
O	GLU	A	2	15.034	-3.194	-2.308	1.00	31.55	8
O	GLU	A	2	13.612	-3.797	-0.734	1.00	31.76	8
C	GLU	A	2	16.475	-1.555	0.338	1.00	39.50	6
O	GLU	A	2	17.517	-1.974	-0.159	1.00	38.79	8
N	TYR	A	2	15.880	-2.163	1.355	1.00	41.62	7
CA	TYR	A	2	16.427	-3.344	1.999	1.00	44.09	6
CB	TYR	A	2	15.416	-3.907	3.007	1.00	47.05	6
C	TYR	A	2	15.966	-5.062	3.815	1.00	51.46	6
C	TYR	A	2	17.060	-4.900	4.653	1.00	53.28	6
CE	TYR	A	2	17.559	-5.961	5.385	1.00	55.01	6
C	TYR	A	2	15.386	-6.320	3.726	1.00	53.44	6
CE	TYR	A	2	15.880	-7.387	4.453	1.00	55.01	6
CZ	TYR	A	2	16.965	-7.200	5.281	1.00	55.79	6
O	TYR	A	2	17.458	-8.260	6.005	1.00	56.98	8
C	TYR	A	2	16.892	-4.439	1.056	1.00	44.36	6
O	TYR	A	2	18.074	-4.800	1.067	1.00	43.99	8
N	GLU	A	2	16.001	-4.973	0.230	1.00	44.51	7
CA	GLU	A	2	16.327	-6.045	-0.699	1.00	45.08	6
CB	GLU	A	2	15.054	-6.560	-1.380	1.00	46.87	6
C	GLU	A	2	14.085	-7.234	-0.421	1.00	49.42	6
C	GLU	A	2	14.666	-8.461	0.254	1.00	50.74	6
O	GLU	A	2	14.917	-9.469	-0.439	1.00	52.14	8
O	GLU	A	2	14.879	-8.424	1.483	1.00	51.57	8
C	GLU	A	2	17.379	-5.678	-1.732	1.00	45.15	6
O	GLU	A	2	18.145	-6.545	-2.162	1.00	45.06	8
N	HIS	A	2	17.454	-4.415	-2.130	1.00	45.19	7
CA	HIS	A	2	18.467	-3.936	-3.055	1.00	45.66	6
CB	HIS	A	2	18.143	-2.502	-3.484	1.00	40.61	6
C	HIS	A	2	19.076	-1.926	-4.501	1.00	35.46	6
C	HIS	A	2	18.978	-1.839	-5.848	1.00	33.88	6
N	HIS	A	2	20.277	-1.340	-4.168	1.00	34.67	7
CE	HIS	A	2	20.886	-0.926	-5.264	1.00	33.14	6
N	HIS	A	2	20.119	-1.219	-6.298	1.00	33.39	7

Figure 1 - 14

C	HIS	A	2	19.852	-3.972	-2.410	1.00	47.38	6
O	HIS	A	2	20.841	-4.346	-3.035	1.00	47.01	8
N	ALA	A	2	19.918	-3.568	-1.146	1.00	49.48	7
CA	ALA	A	2	21.156	-3.512	-0.387	1.00	51.58	6
CB	ALA	A	2	20.957	-2.642	0.850	1.00	50.94	6
C	ALA	A	2	21.672	-4.883	0.025	1.00	53.16	6
O	ALA	A	2	22.872	-5.150	-0.033	1.00	53.00	8
N	LYS	A	2	20.762	-5.756	0.439	1.00	55.23	7
CA	LYS	A	2	21.119	-7.119	0.829	1.00	57.65	6
CB	LYS	A	2	19.908	-7.816	1.441	1.00	60.63	6
C	LYS	A	2	20.032	-9.315	1.639	1.00	65.05	6
C	LYS	A	2	18.678	-9.947	1.929	1.00	67.78	6
CE	LYS	A	2	18.832	-	2.540	1.00	69.75	6
NZ	LYS	A	2	17.937	-	3.715	1.00	71.19	7
C	LYS	A	2	21.651	-7.883	-0.379	1.00	58.57	6
O	LYS	A	2	22.648	-8.601	-0.295	1.00	59.09	8
N	LYS	A	2	21.013	-7.719	-1.532	1.00	59.06	7
CA	LYS	A	2	21.396	-8.367	-2.775	1.00	59.54	6
CB	LYS	A	2	20.417	-7.977	-3.889	1.00	61.74	6
C	LYS	A	2	20.739	-8.548	-5.257	1.00	64.55	6
C	LYS	A	2	19.526	-8.538	-6.174	1.00	67.02	6
CE	LYS	A	2	18.684	-9.790	-5.989	1.00	67.96	6
NZ	LYS	A	2	17.562	-9.562	-5.037	1.00	69.74	7
C	LYS	A	2	22.823	-8.063	-3.209	1.00	59.47	6
O	LYS	A	2	23.481	-8.928	-3.797	1.00	59.77	8
N	ARG	A	2	23.316	-6.854	-2.971	1.00	59.19	7
CA	ARG	A	2	24.684	-6.494	-3.318	1.00	58.96	6
CB	ARG	A	2	24.750	-5.060	-3.845	1.00	64.49	6
C	ARG	A	2	24.662	-4.964	-5.361	1.00	70.34	6
C	ARG	A	2	23.628	-3.938	-5.797	1.00	75.18	6
N	ARG	A	2	22.590	-4.519	-6.639	1.00	79.23	7
CZ	ARG	A	2	21.967	-3.901	-7.633	1.00	81.69	6
N	ARG	A	2	22.262	-2.646	-7.948	1.00	83.33	7
N	ARG	A	2	21.033	-4.539	-8.329	1.00	82.48	7
C	ARG	A	2	25.622	-6.683	-2.129	1.00	57.70	6
O	ARG	A	2	26.843	-6.647	-2.276	1.00	57.09	8
N	GLY	A	2	25.063	-6.888	-0.942	1.00	56.76	7
CA	GLY	A	2	25.818	-7.122	0.271	1.00	55.73	6
C	GLY	A	2	26.477	-5.887	0.860	1.00	55.04	6
O	GLY	A	2	27.669	-5.896	1.171	1.00	55.17	8
N	ALA	A	2	25.704	-4.826	1.051	1.00	54.08	7
CA	ALA	A	2	26.217	-3.573	1.579	1.00	52.80	6
CB	ALA	A	2	25.297	-2.438	1.128	1.00	52.47	6
C	ALA	A	2	26.349	-3.532	3.095	1.00	51.83	6
O	ALA	A	2	25.664	-4.236	3.829	1.00	51.72	8
N	LYS	A	2	27.193	-2.616	3.565	1.00	51.12	7
CA	LYS	A	2	27.295	-2.288	4.982	1.00	50.26	6
CB	LYS	A	2	28.369	-1.226	5.205	1.00	53.24	6
C	LYS	A	2	29.768	-1.712	5.519	1.00	56.48	6
C	LYS	A	2	30.667	-0.551	5.931	1.00	58.30	6
CE	LYS	A	2	31.652	-0.193	4.830	1.00	60.07	6
NZ	LYS	A	2	32.926	-0.955	4.954	1.00	60.39	7
C	LYS	A	2	25.952	-1.720	5.445	1.00	48.90	6
O	LYS	A	2	25.615	-0.610	5.024	1.00	49.32	8
N	ILE	A	2	25.198	-2.448	6.257	1.00	47.08	7
CA	ILE	A	2	23.908	-1.931	6.720	1.00	45.16	6
CB	ILE	A	2	22.789	-2.978	6.630	1.00	47.32	6
C	ILE	A	2	21.571	-2.590	7.459	1.00	48.62	6
C	ILE	A	2	22.379	-3.171	5.165	1.00	48.61	6
C	ILE	A	2	21.380	-4.277	4.914	1.00	49.33	6
C	ILE	A	2	24.061	-1.379	8.132	1.00	43.27	6
O	ILE	A	2	24.130	-2.120	9.109	1.00	43.57	8
N	TYR	A	2	24.085	-0.055	8.243	1.00	40.91	7
CA	TYR	A	2	24.251	0.633	9.510	1.00	38.29	6

C	CB	TYR	A	2	24.564	2.118	9.276	1.00	36.36	6
C	C	TYR	A	2	25.973	2.410	8.826	1.00	33.88	6
C	C	TYR	A	2	26.265	2.576	7.480	1.00	33.29	6
CE	C	TYR	A	2	27.553	2.850	7.058	1.00	33.19	6
C	C	TYR	A	2	27.007	2.532	9.744	1.00	32.95	6
CE	C	TYR	A	2	28.298	2.805	9.331	1.00	32.34	6
CZ	C	TYR	A	2	28.562	2.963	7.990	1.00	32.93	6
O	C	TYR	A	2	29.843	3.235	7.572	1.00	33.91	8
C	O	TYR	A	2	23.010	0.588	10.393	1.00	37.77	6
O	N	TYR	A	2	23.112	0.610	11.619	1.00	37.81	8
N	CA	ALA	A	2	21.839	0.629	9.769	1.00	37.28	7
CA	CB	ALA	A	2	20.581	0.637	10.500	1.00	36.62	6
CB	C	ALA	A	2	20.556	1.758	11.528	1.00	37.87	6
C	O	ALA	A	2	19.407	0.791	9.536	1.00	36.09	6
O	N	ALA	A	2	19.578	0.861	8.320	1.00	35.78	8
N	CA	GLU	A	2	18.214	0.845	10.109	1.00	35.82	7
CA	CB	GLU	A	2	16.988	0.971	9.338	1.00	35.66	6
CB	C	GLU	A	2	16.120	-0.270	9.577	1.00	37.13	6
C	O	GLU	A	2	14.914	-0.407	8.670	1.00	40.33	6
C	O	GLU	A	2	14.032	-1.593	8.998	1.00	41.53	6
O	C	GLU	A	2	12.858	-1.611	8.569	1.00	42.20	8
O	C	GLU	A	2	14.495	-2.527	9.684	1.00	44.11	8
C	O	GLU	A	2	16.206	2.219	9.719	1.00	35.25	6
O	N	GLU	A	2	16.047	2.517	10.903	1.00	35.55	8
N	CA	LEU	A	2	15.720	2.940	8.714	1.00	35.26	7
CA	CB	LEU	A	2	14.875	4.109	8.973	1.00	35.14	6
CB	C	LEU	A	2	14.941	5.121	7.842	1.00	37.51	6
C	O	LEU	A	2	14.734	6.596	8.200	1.00	38.88	6
C	O	LEU	A	2	14.959	7.476	6.980	1.00	39.79	6
C	O	LEU	A	2	13.347	6.835	8.775	1.00	39.55	6
C	O	LEU	A	2	13.459	3.548	9.133	1.00	34.67	6
O	N	LEU	A	2	12.973	2.920	8.188	1.00	34.29	8
N	CA	VAL	A	2	12.895	3.592	10.335	1.00	34.72	7
CA	CB	VAL	A	2	11.617	2.935	10.582	1.00	34.44	6
CB	C	VAL	A	2	11.705	1.917	11.743	1.00	34.57	6
C	O	VAL	A	2	12.615	0.751	11.386	1.00	34.70	6
C	O	VAL	A	2	12.178	2.591	13.021	1.00	33.08	6
C	O	VAL	A	2	10.470	3.886	10.886	1.00	34.39	6
O	N	VAL	A	2	9.314	3.451	10.859	1.00	34.63	8
N	CA	GLY	A	2	10.762	5.143	11.202	1.00	33.88	7
CA	CB	GLY	A	2	9.705	6.096	11.517	1.00	33.36	6
C	O	GLY	A	2	10.056	7.521	11.115	1.00	33.06	6
O	N	GLY	A	2	11.207	7.948	11.198	1.00	32.88	8
N	CA	PHE	A	2	9.045	8.266	10.676	1.00	32.28	7
CA	CB	PHE	A	2	9.210	9.662	10.292	1.00	31.30	6
CB	C	PHE	A	2	9.510	9.826	8.806	1.00	28.59	6
C	O	PHE	A	2	9.670	11.243	8.332	1.00	26.83	6
C	O	PHE	A	2	10.350	12.190	9.078	1.00	25.03	6
C	O	PHE	A	2	9.142	11.628	7.107	1.00	26.91	6
CE	C	PHE	A	2	10.483	13.492	8.636	1.00	23.91	6
CE	C	PHE	A	2	9.283	12.923	6.648	1.00	27.39	6
CZ	C	PHE	A	2	9.956	13.857	7.415	1.00	25.55	6
C	O	PHE	A	2	7.959	10.450	10.674	1.00	30.86	6
O	N	PHE	A	2	6.861	10.129	10.222	1.00	31.29	8
N	CA	GLY	A	2	8.133	11.468	11.508	1.00	30.72	7
CA	CB	GLY	A	2	7.022	12.288	11.963	1.00	30.39	6
C	O	GLY	A	2	7.260	13.770	11.707	1.00	30.81	6
O	N	GLY	A	2	8.373	14.278	11.829	1.00	30.69	8
N	CA	MET	A	2	6.197	14.471	11.324	1.00	30.70	7
CA	CB	MET	A	2	6.247	15.891	11.031	1.00	30.12	6
CB	C	MET	A	2	6.123	16.172	9.536	1.00	29.88	6
C	O	MET	A	2	7.226	15.696	8.618	1.00	29.92	6
SD	C	MET	A	2	6.633	15.492	6.924	1.00	34.18	1
CE	C	MET	A	2	6.376	17.202	6.467	1.00	37.05	6

Figure 1 - 15

C	LEU	A	2	0.415	18.015	16.133	1.00	40.11	6
C	LEU	A	2	0.639	15.522	16.125	1.00	41.11	6
C	LEU	A	2	4.007	15.066	16.966	1.00	34.13	6
O	LEU	A	2	3.695	13.968	16.499	1.00	33.81	8
N	ALA	A	2	5.152	15.667	16.648	1.00	33.82	7
CA	ALA	A	2	6.119	15.068	15.736	1.00	33.23	6
CB	ALA	A	2	7.212	16.070	15.395	1.00	32.79	6
C	ALA	A	2	6.713	13.783	16.305	1.00	32.82	6
O	ALA	A	2	6.930	12.826	15.555	1.00	31.82	8
N	MET	A	2	6.969	13.751	17.614	1.00	32.44	7
CA	MET	A	2	7.455	12.516	18.239	1.00	32.54	6
CB	MET	A	2	7.999	12.771	19.636	1.00	32.06	6
C	MET	A	2	9.285	13.590	19.637	1.00	30.75	6
SD	MET	A	2	10.047	13.718	21.262	1.00	31.85	1
CE	MET	A	2	9.278	15.202	21.899	1.00	24.03	6
C	MET	A	2	6.317	11.502	18.214	1.00	32.99	6
O	MET	A	2	6.464	10.387	17.711	1.00	33.07	8
N	ALA	A	2	5.123	11.934	18.613	1.00	33.83	7
CA	ALA	A	2	3.931	11.100	18.540	1.00	34.86	6
CB	ALA	A	2	2.696	11.897	18.938	1.00	36.22	6
C	ALA	A	2	3.739	10.514	17.145	1.00	35.40	6
O	ALA	A	2	3.541	9.302	17.030	1.00	36.47	8
N	ASN	A	2	3.817	11.328	16.094	1.00	35.07	7
CA	ASN	A	2	3.628	10.851	14.733	1.00	34.90	6
CB	ASN	A	2	3.547	12.010	13.730	1.00	36.26	6
C	ASN	A	2	2.252	12.789	13.851	1.00	38.25	6
O	ASN	A	2	1.213	12.236	14.216	1.00	38.80	8
N	ASN	A	2	2.304	14.081	13.551	1.00	37.08	7
C	ASN	A	2	4.695	9.867	14.279	1.00	34.23	6
O	ASN	A	2	4.368	8.877	13.619	1.00	34.76	8
N	ALA	A	2	5.960	10.112	14.603	1.00	33.99	7
CA	ALA	A	2	7.040	9.208	14.218	1.00	33.42	6
CB	ALA	A	2	8.390	9.816	14.556	1.00	32.45	6
C	ALA	A	2	6.871	7.856	14.905	1.00	33.89	6
O	ALA	A	2	7.067	6.797	14.309	1.00	33.23	8
N	LEU	A	2	6.505	7.889	16.183	1.00	34.57	7
CA	LEU	A	2	6.198	6.693	16.953	1.00	35.73	6
CB	LEU	A	2	5.749	7.072	18.366	1.00	36.10	6
C	LEU	A	2	6.828	7.524	19.350	1.00	36.96	6
C	LEU	A	2	6.202	7.916	20.681	1.00	36.30	6
C	LEU	A	2	7.876	6.440	19.560	1.00	38.05	6
C	LEU	A	2	5.109	5.871	16.271	1.00	36.49	6
O	LEU	A	2	5.281	4.682	16.001	1.00	36.03	8
N	ARG	A	2	3.990	6.518	15.949	1.00	37.50	7
CA	ARG	A	2	2.879	5.857	15.266	1.00	38.38	6
CB	ARG	A	2	1.704	6.821	15.124	1.00	43.58	6
C	ARG	A	2	0.688	6.482	14.048	1.00	49.95	6
C	ARG	A	2	-0.490	7.442	14.066	1.00	55.15	6
N	ARG	A	2	-0.190	8.707	13.			

CB	ALA	A	2	8.334	3.400	14.135	1.00	42.87	6
C	ALA	A	2	6.335	1.908	13.964	1.00	42.62	6
O	ALA	A	2	6.650	0.731	13.796	1.00	43.14	8
N	GLY	A	2	5.304	2.271	14.719	1.00	43.20	7
CA	GLY	A	2	4.452	1.297	15.387	1.00	43.62	6
C	GLY	A	2	5.114	0.739	16.638	1.00	43.92	6
O	GLY	A	2	5.107	-0.466	16.884	1.00	44.21	8
N	ILE	A	2	5.771	1.613	17.390	1.00	43.72	7
CA	ILE	A	2	6.425	1.245	18.635	1.00	43.55	6
CB	ILE	A	2	7.958	1.199	18.545	1.00	42.75	6
C	ILE	A	2	8.444	-0.071	17.859	1.00	41.52	6
C	ILE	A	2	8.506	2.431	17.820	1.00	42.54	6
C	ILE	A	2	9.940	2.759	18.178	1.00	43.11	6
C	ILE	A	2	6.023	2.261	19.704	1.00	43.86	6
O	ILE	A	2	5.637	3.378	19.357	1.00	43.43	8
N	GLU	A	2	6.097	1.867	20.968	1.00	45.03	7
CA	GLU	A	2	5.758	2.805	22.040	1.00	46.66	6
CB	GLU	A	2	5.132	2.074	23.223	1.00	53.41	6
C	GLU	A	2	3.772	1.466	22.905	1.00	60.11	6
C	GLU	A	2	2.955	1.176	24.149	1.00	64.17	6
O	GLU	A	2	2.576	0.003	24.354	1.00	66.12	8
O	GLU	A	2	2.690	2.121	24.922	1.00	66.54	8
C	GLU	A	2	7.005	3.582	22.436	1.00	46.19	6
O	GLU	A	2	8.121	3.206	22.071	1.00	45.77	8
N	ALA	A	2	6.845	4.639	23.220	1.00	46.33	7
CA	ALA	A	2	7.948	5.479	23.657	1.00	46.88	6
CB	ALA	A	2	7.386	6.701	24.387	1.00	45.93	6
C	ALA	A	2	8.978	4.794	24.538	1.00	47.23	6
O	ALA	A	2	10.126	5.249	24.609	1.00	47.89	8
N	SER	A	2	8.656	3.686	25.190	1.00	47.44	7
CA	SER	A	2	9.558	2.956	26.061	1.00	47.10	6
CB	SER	A	2	8.742	2.180	27.106	1.00	48.58	6
O	SER	A	2	8.071	1.092	26.492	1.00	49.60	8
C	SER	A	2	10.487	1.993	25.337	1.00	46.51	6
O	SER	A	2	11.244	1.248	25.965	1.00	47.13	8
N	GLN	A	2	10.457	1.987	24.013	1.00	45.51	7
CA	GLN	A	2	11.310	1.141	23.192	1.00	43.84	6
CB	GLN	A	2	10.514	0.498	22.058	1.00	45.59	6
C	GLN	A	2	9.657	-0.671	22.514	1.00	48.22	6
C	GLN	A	2	8.571	-1.048	21.531	1.00	50.32	6
O	GLN	A	2	8.830	-1.682	20.506	1.00	51.41	8
N	GLN	A	2	7.336	-0.664	21.837	1.00	51.31	7
C	GLN	A	2	12.472	1.979	22.658	1.00	42.12	6
O	GLN	A	2	13.417	1.474	22.059	1.00	41.78	8
N	ILE	A	2	12.397	3.283	22.904	1.00	40.51	7
CA	ILE	A	2	13.436	4.222	22.523	1.00	39.86	6
CB	ILE	A	2	12.873	5.622	22.207	1.00	40.19	6
C	ILE	A	2	13.992	6.609	21.897	1.00	39.47	6
C	ILE	A	2	11.861	5.567	21.063	1.00	40.86	6
C	ILE	A	2	12.417	5.221	19.702	1.00	40.33	6
C	ILE	A	2	14.466	4.359	23.644	1.00	39.12	6
O	ILE	A	2	14.144	4.781	24.753	1.00	39.07	8
N	GLY	A	2	15.712	4.023	23.335	1.00	38.94	7
CA	GLY	A	2	16.789	4.127	24.309	1.00	38.40	6
C	GLY	A	2	17.317	5.557	24.385	1.00	38.27	6
O	GLY	A	2	17.438	6.113	25.478	1.00	39.05	8
N	TYR	A	2	17.608	6.152	23.231	1.00	37.49	7
CA	TYR	A	2	18.231	7.471	23.206	1.00	36.85	6
CB	TYR	A	2	19.714	7.308	22.877	1.00	36.62	6
C	TYR	A	2	20.474	8.536	22.443	1.00	36.28	6
C	TYR	A	2	21.036	8.603	21.173	1.00	36.11	6
CE	TYR	A	2	21.745	9.715	20.759	1.00	35.70	6
C	TYR	A	2	20.650	9.621	23.290	1.00	36.10	6
CE	TYR	A	2	21.362	10.736	22.887	1.00	36.03	6

Figure 1 - 17

C	VAL	A	3	11.856	14.898	25.087	1.00	46.70	6
C	VAL	A	3	8.919	13.883	27.364	1.00	47.82	6
O	VAL	A	3	8.604	12.693	27.365	1.00	47.71	8
N	LYS	A	3	8.585	14.714	28.349	1.00	48.07	7
CA	LYS	A	3	7.799	14.263	29.494	1.00	48.68	6
CB	LYS	A	3	7.654	15.386	30.523	1.00	48.79	6
C	LYS	A	3	8.880	15.539	31.412	1.00	49.95	6
C	LYS	A	3	8.716	16.660	32.425	1.00	51.90	6
CE	LYS	A	3	9.831	16.618	33.459	1.00	53.93	6
NZ	LYS	A	3	9.808	17.806	34.357	1.00	55.89	7
C	LYS	A	3	6.439	13.762	29.024	1.00	49.02	6
O	LYS	A	3	6.044	12.632	29.302	1.00	49.46	8
N	THR	A	3	5.771	14.551	28.192	1.00	48.90	7
CA	THR	A	3	4.469	14.237	27.636	1.00	49.03	6
CB	THR	A	3	3.972	15.427	26.782	1.00	48.10	6
O	THR	A	3	4.097	16.635	27.549	1.00	47.21	8
C	THR	A	3	2.522	15.250	26.372	1.00	46.85	6
C	THR	A	3	4.411	12.968	26.804	1.00	49.57	6
O	THR	A	3	3.380	12.285	26.804	1.00	50.05	8
N	ILE	A	3	5.462	12.637	26.068	1.00	50.18	7
CA	ILE	A	3	5.470	11.469	25.198	1.00	50.51	6
CB	ILE	A	3	6.342	11.746	23.954	1.00	50.53	6
C	ILE	A	3	6.438	10.528	23.051	1.00	50.20	6
C	ILE	A	3	5.800	12.953	23.183	1.00	51.45	6
C	ILE	A	3	4.379	12.825	22.680	1.00	51.49	6
C	ILE	A	3	5.936	10.194	25.880	1.00	50.83	6
O	ILE	A	3	5.339	9.134	25.668	1.00	50.86	8
N	PHE	A	3	7.014	10.262	26.651	1.00	51.33	7
CA	PHE	A	3	7.560	9.065	27.288	1.00	52.19	6
CB	PHE	A	3	9.074	9.195	27.452	1.00	52.50	6
C	PHE	A	3	9.821	9.238	26.147	1.00	53.33	6
C	PHE	A	3	9.830	10.383	25.370	1.00	53.36	6
C	PHE	A	3	10.525	8.132	25.702	1.00	53.23	6
CE	PHE	A	3	10.516	10.426	24.173	1.00	53.94	6
CE	PHE	A	3	11.217	8.168	24.507	1.00	54.53	6
CZ	PHE	A	3	11.213	9.316	23.740	1.00	54.18	6
C	PHE	A	3	6.871	8.762	28.610	1.00	52.24	6
O	PHE	A	3	6.695	7.597	28.973	1.00	51.99	8
N	GLY	A	3	6.444	9.798	29.320	1.00	52.78	7
CA	GLY	A	3	5.693	9.654	30.551	1.00	53.77	6
C	GLY	A	3	6.446	8.986	31.687	1.00	54.34	6
O	GLY	A	3	7.227	9.630	32.388	1.00	54.23	8
N	GLU	A	3	6.205	7.690	31.888	1.00	54.80	7
CA	GLU	A	3	6.838	6.949	32.975	1.00	55.28	6
CB	GLU	A	3	5.960	5.789	33.443	1.00	58.98	6
C	GLU	A	3	4.949	6.181	34.517	1.00	62.90	6
C	GLU	A	3	3.537	6.208	33.959	1.00	65.17	6
O	GLU	A	3	3.089	7.295	33.536	1.00	67.07	8
O	GLU	A	3	2.888					

O	SER	A	3	12.171	8.052	35.359	1.00	57.76	8
C	SER	A	3	14.399	7.821	33.107	1.00	56.08	6
O	SER	A	3	15.603	7.733	33.355	1.00	56.24	8
N	ARG	A	3	13.781	6.902	32.386	1.00	56.22	7
CA	ARG	A	3	14.416	5.726	31.814	1.00	56.26	6
CB	ARG	A	3	13.344	4.651	31.647	1.00	61.19	6
C	ARG	A	3	13.701	3.372	30.920	1.00	66.66	6
C	ARG	A	3	12.447	2.526	30.737	1.00	71.39	6
N	ARG	A	3	12.695	1.230	30.126	1.00	75.06	7
CZ	ARG	A	3	11.756	0.312	29.913	1.00	77.16	6
N	ARG	A	3	10.497	0.540	30.262	1.00	78.29	7
N	ARG	A	3	12.073	-0.845	29.347	1.00	78.92	7
C	ARG	A	3	15.110	6.023	30.491	1.00	55.03	6
O	ARG	A	3	16.028	5.296	30.105	1.00	55.13	8
N	VAL	A	3	14.705	7.077	29.789	1.00	53.57	7
CA	VAL	A	3	15.284	7.424	28.496	1.00	51.50	6
CB	VAL	A	3	14.174	7.860	27.515	1.00	51.84	6
C	VAL	A	3	13.523	9.165	27.947	1.00	51.31	6
C	VAL	A	3	14.710	7.972	26.095	1.00	51.08	6
C	VAL	A	3	16.377	8.479	28.545	1.00	49.96	6
O	VAL	A	3	16.278	9.497	29.227	1.00	50.25	8
N	LEU	A	3	17.436	8.250	27.770	1.00	48.09	7
CA	LEU	A	3	18.567	9.163	27.688	1.00	45.94	6
CB	LEU	A	3	19.875	8.398	27.483	1.00	43.63	6
C	LEU	A	3	20.080	7.094	28.254	1.00	43.75	6
C	LEU	A	3	21.455	6.510	27.955	1.00	41.34	6
C	LEU	A	3	19.912	7.299	29.751	1.00	42.51	6
C	LEU	A	3	18.397	10.184	26.566	1.00	44.92	6
O	LEU	A	3	18.184	9.849	25.402	1.00	44.57	8
N	VAL	A	3	18.446	11.460	26.934	1.00	43.75	7
CA	VAL	A	3	18.292	12.568	26.006	1.00	42.60	6
CB	VAL	A	3	17.056	13.434	26.333	1.00	42.79	6
C	VAL	A	3	16.914	14.564	25.318	1.00	43.51	6
C	VAL	A	3	15.771	12.628	26.391	1.00	41.10	6
C	VAL	A	3	19.511	13.487	26.057	1.00	41.36	6
O	VAL	A	3	19.660	14.195	27.055	1.00	41.26	8
N	SER	A	3	20.277	13.602	24.978	1.00	40.10	7
CA	SER	A	3	21.417	14.515	24.995	1.00	38.23	6
CB	SER	A	3	22.726	13.733	25.111	1.00	38.48	6
O	SER	A	3	23.125	13.209	23.860	1.00	37.54	8
C	SER	A	3	21.462	15.432	23.779	1.00	37.10	6
O	SER	A	3	20.980	15.110	22.696	1.00	36.20	8
N	SER	A	3	22.080	16.597	23.971	1.00	36.01	7
CA	SER	A	3	22.287	17.541	22.882	1.00	34.31	6
CB	SER	A	3	21.798	18.939	23.261	1.00	34.82	6
O	SER	A	3	22.083	19.885	22.245	1.00	31.05	8
C	SER	A	3	23.762	17.580	22.501	1.00	33.61	6
O	SER	A	3	24.597	18.118	23.233	1.00	33.03	8
N	THR	A	3	24.072	17.129	21.284	1.00	32.62	7
CA	THR	A	3	25.437	17.172	20.775	1.00	32.08	6
CB	THR	A	3	25.726	16.101	19.712	1.00	33.01	6
O	THR	A	3	24.747	16.143	18.667	1.00	34.86	8
C	THR	A	3	25.711	14.716	20.347	1.00	32.74	6
C	THR	A	3	25.793	18.553	20.240	1.00	31.64	6
O	THR	A	3	26.924	18.826	19.840	1.00	31.14	8
N	LYS	A	3	24.856	19.491	20.300	1.00	31.31	7
CA	LYS	A	3	25.010	20.881	19.939	1.00	31.62	6
CB	LYS	A	3	23.654	21.553	19.710	1.00	29.29	6
C	LYS	A	3	22.892	21.070	18.485	1.00	26.40	6
C	LYS	A	3	21.836	22.083	18.071	1.00	26.12	6
CE	LYS	A	3	21.019	21.625	16.880	1.00	19.32	6
NZ	LYS	A	3	20.357	20.315	17.079	1.00	19.99	7
C	LYS	A	3	25.777	21.650	21.017	1.00	32.18	6
O	LYS	A	3	26.227	22.774	20.790	1.00	31.78	8

N	SER	A	3	26.013	21.033	22.170	1.00	32.16	7
CA	SER	A	3	26.870	21.550	23.217	1.00	32.60	6
CB	SER	A	3	26.670	20.797	24.533	1.00	33.17	6
O	SER	A	3	26.705	19.395	24.356	1.00	33.68	8
C	SER	A	3	28.342	21.501	22.812	1.00	32.18	6
O	SER	A	3	29.145	22.294	23.305	1.00	32.58	8
N	MET	A	3	28.707	20.593	21.918	1.00	31.37	7
CA	MET	A	3	30.066	20.471	21.421	1.00	30.45	6
CB	MET	A	3	30.467	18.989	21.389	1.00	29.91	6
C	MET	A	3	30.627	18.359	22.763	1.00	30.11	6
SD	MET	A	3	30.676	16.559	22.727	1.00	27.38	1
CE	MET	A	3	28.930	16.174	22.612	1.00	28.29	6
C	MET	A	3	30.209	21.045	20.013	1.00	29.74	6
O	MET	A	3	31.181	21.695	19.643	1.00	30.42	8
N	THR	A	3	29.206	20.776	19.194	1.00	28.53	7
CA	THR	A	3	29.221	21.052	17.764	1.00	26.82	6
CB	THR	A	3	28.529	19.849	17.084	1.00	25.06	6
O	THR	A	3	29.276	19.446	15.930	1.00	30.10	8
C	THR	A	3	27.090	20.114	16.701	1.00	18.67	6
C	THR	A	3	28.614	22.391	17.399	1.00	26.37	6
O	THR	A	3	29.054	23.058	16.457	1.00	26.07	8
N	GLY	A	3	27.618	22.819	18.170	1.00	25.19	7
CA	GLY	A	3	26.920	24.078	17.903	1.00	23.14	6
C	GLY	A	3	25.703	23.739	17.033	1.00	22.02	6
O	GLY	A	3	25.454	22.562	16.775	1.00	20.89	8
N	HIS	A	3	24.951	24.734	16.597	1.00	21.15	7
CA	HIS	A	3	23.784	24.482	15.756	1.00	21.64	6
CB	HIS	A	3	22.651	25.433	16.132	1.00	22.64	6
C	HIS	A	3	21.345	25.179	15.448	1.00	22.18	6
C	HIS	A	3	20.906	24.174	14.655	1.00	22.76	6
N	HIS	A	3	20.290	26.062	15.559	1.00	21.82	7
CE	HIS	A	3	19.267	25.608	14.868	1.00	22.80	6
N	HIS	A	3	19.610	24.462	14.307	1.00	22.54	7
C	HIS	A	3	24.154	24.629	14.285	1.00	21.46	6
O	HIS	A	3	24.436	25.735	13.825	1.00	20.69	8
N	LEU	A	3	24.046	23.547	13.518	1.00	21.57	7
CA	LEU	A	3	24.414	23.543	12.110	1.00	21.84	6
CB	LEU	A	3	25.023	22.217	11.684	1.00	23.76	6
C	LEU	A	3	26.176	21.514	12.363	1.00	26.89	6
C	LEU	A	3	27.099	20.895	11.311	1.00	23.94	6
C	LEU	A	3	26.984	22.392	13.303	1.00	26.29	6
C	LEU	A	3	23.230	23.833	11.187	1.00	21.61	6
O	LEU	A	3	23.245	23.478	10.007	1.00	20.96	8
N	LEU	A	3	22.196	24.471	11.711	1.00	21.90	7
CA	LEU	A	3	21.000	24.829	10.971	1.00	20.97	6
CB	LEU	A	3	21.256	26.146	10.227	1.00	25.02	6
C	LEU	A	3	21.228	27.387	11.132	1.00	29.21	6
C	LEU	A	3	21.823	28.592	10.425	1.0		

O	ALA	A	3	21.709	17.524	12.734	1.00	18.70	8
N	GLY	A	3	20.093	18.284	11.392	1.00	18.49	7
CA	GLY	A	3	19.346	17.044	11.340	1.00	18.89	6
C	GLY	A	3	20.085	15.914	10.641	1.00	19.95	6
O	GLY	A	3	19.804	14.742	10.908	1.00	20.23	8
N	ALA	A	3	20.979	16.235	9.714	1.00	20.89	7
CA	ALA	A	3	21.739	15.234	8.980	1.00	22.22	6
CB	ALA	A	3	22.286	15.830	7.690	1.00	20.29	6
C	ALA	A	3	22.879	14.657	9.815	1.00	23.42	6
O	ALA	A	3	22.998	13.436	9.944	1.00	22.82	8
N	VAL	A	3	23.692	15.528	10.413	1.00	23.70	7
CA	VAL	A	3	24.804	15.087	11.243	1.00	24.94	6
CB	VAL	A	3	25.732	16.231	11.691	1.00	24.96	6
C	VAL	A	3	26.375	16.906	10.489	1.00	24.13	6
C	VAL	A	3	25.004	17.259	12.543	1.00	24.96	6
C	VAL	A	3	24.313	14.344	12.482	1.00	25.74	6
O	VAL	A	3	24.898	13.344	12.896	1.00	25.66	8
N	GLU	A	3	23.217	14.813	13.064	1.00	26.47	7
CA	GLU	A	3	22.620	14.235	14.251	1.00	27.57	6
CB	GLU	A	3	21.656	15.256	14.879	1.00	24.46	6
C	GLU	A	3	22.395	16.436	15.485	1.00	22.46	6
C	GLU	A	3	21.493	17.567	15.920	1.00	21.93	6
O	GLU	A	3	20.285	17.356	16.143	1.00	25.13	8
O	GLU	A	3	22.008	18.695	16.057	1.00	23.51	8
C	GLU	A	3	21.897	12.920	14.010	1.00	28.69	6
O	GLU	A	3	21.691	12.158	14.960	1.00	29.70	8
N	SER	A	3	21.511	12.638	12.770	1.00	28.70	7
CA	SER	A	3	20.966	11.335	12.408	1.00	28.87	6
CB	SER	A	3	20.299	11.349	11.037	1.00	29.67	6
O	SER	A	3	19.060	12.029	11.055	1.00	30.09	8
C	SER	A	3	22.102	10.311	12.417	1.00	28.45	6
O	SER	A	3	21.917	9.172	12.834	1.00	29.17	8
N	ILE	A	3	23.279	10.741	11.973	1.00	28.01	7
CA	ILE	A	3	24.466	9.891	11.972	1.00	28.28	6
CB	ILE	A	3	25.635	10.555	11.223	1.00	27.00	6
C	ILE	A	3	26.906	9.724	11.315	1.00	24.00	6
C	ILE	A	3	25.237	10.769	9.761	1.00	25.93	6
C	ILE	A	3	26.150	11.648	8.942	1.00	25.92	6
C	ILE	A	3	24.857	9.551	13.407	1.00	28.54	6
O	ILE	A	3	24.990	8.374	13.750	1.00	29.30	8
N	TYR	A	3	24.886	10.547	14.288	1.00	27.81	7
CA	TYR	A	3	25.154	10.328	15.705	1.00	27.86	6
CB	TYR	A	3	25.121	11.625	16.505	1.00	25.65	6
C	TYR	A	3	25.927	12.780	15.961	1.00	23.07	6
C	TYR	A	3	25.562	14.087	16.265	1.00	21.60	6
CE	TYR	A	3	26.286	15.162	15.788	1.00	21.08	6
C	TYR	A	3	27.047	12.591	15.162	1.00	22.29	6
CE	TYR	A	3	27.769	13.657	14.670	1.00	22.16	6
CZ	TYR	A	3	27.385	14.942	14.990	1.00	21.49	6
O	TYR	A	3	28.109	16.006	14.503	1.00	22.00	8
C	TYR	A	3	24.163	9.331	16.298	1.00	28.50	6
O	TYR	A	3	24.562	8.399	16.999	1.00	29.32	8
N	SER	A	3	22.883	9.476	15.971	1.00	28.28	7
CA	SER	A	3	21.853	8.550	16.415	1.00	28.66	6
CB	SER	A	3	20.471	9.074	16.017	1.00	26.37	6
O	SER	A	3	20.239	10.351	16.586	1.00	24.94	8
C	SER	A	3	22.059	7.145	15.858	1.00	29.49	6
O	SER	A	3	21.716	6.164	16.523	1.00	29.71	8
N	ILE	A	3	22.581	7.026	14.644	1.00	29.91	7
CA	ILE	A	3	22.871	5.731	14.041	1.00	30.85	6
CB	ILE	A	3	23.042	5.854	12.518	1.00	29.44	6
C	ILE	A	3	23.695	4.632	11.898	1.00	24.70	6
C	ILE	A	3	21.671	6.100	11.866	1.00	30.99	6
C	ILE	A	3	21.746	6.717	10.487	1.00	31.70	6

Figure 1 - 20

C	ILE	A	3	24.097	5.109	14.695	1.00	32.09	6
O	ILE	A	3	24.031	3.988	15.209	1.00	33.13	8
N	LEU	A	3	25.190	5.860	14.785	1.00	32.34	7
CA	LEU	A	3	26.426	5.390	15.399	1.00	32.59	6
CB	LEU	A	3	27.530	6.448	15.295	1.00	29.08	6
C	LEU	A	3	27.995	6.776	13.872	1.00	28.35	6
C	LEU	A	3	28.988	7.929	13.881	1.00	25.33	6
C	LEU	A	3	28.590	5.552	13.191	1.00	25.41	6
C	LEU	A	3	26.230	4.952	16.840	1.00	33.29	6
O	LEU	A	3	26.799	3.947	17.275	1.00	32.95	8
N	ALA	A	3	25.381	5.648	17.590	1.00	34.07	7
CA	ALA	A	3	25.047	5.296	18.959	1.00	35.50	6
CB	ALA	A	3	24.015	6.269	19.512	1.00	32.60	6
C	ALA	A	3	24.517	3.866	19.051	1.00	36.95	6
O	ALA	A	3	24.828	3.188	19.996	1.00	37.29	8
N	LEU	A	3	23.718	3.445	18.076	1.00	38.32	7
CA	LEU	A	3	23.214	2.088	17.983	1.00	39.35	6
CB	LEU	A	3	22.126	1.997	16.905	1.00	38.88	6
C	LEU	A	3	20.818	2.741	17.188	1.00	39.57	6
C	LEU	A	3	19.876	2.632	15.997	1.00	38.00	6
C	LEU	A	3	20.150	2.219	18.451	1.00	37.64	6
C	LEU	A	3	24.309	1.071	17.680	1.00	40.04	6
O	LEU	A	3	24.264	-0.056	18.179	1.00	40.72	8
N	ARG	A	3	25.284	1.444	16.859	1.00	39.72	7
CA	ARG	A	3	26.374	0.555	16.489	1.00	39.68	6
CB	ARG	A	3	27.145	1.143	15.299	1.00	38.11	6
C	ARG	A	3	28.395	0.374	14.912	1.00	36.96	6
C	ARG	A	3	29.233	1.118	13.887	1.00	35.78	6
N	ARG	A	3	30.059	2.153	14.494	1.00	36.32	7
CZ	ARG	A	3	31.013	2.835	13.874	1.00	35.89	6
N	ARG	A	3	31.282	2.612	12.595	1.00	35.44	7
N	ARG	A	3	31.700	3.756	14.537	1.00	37.40	7
C	ARG	A	3	27.347	0.292	17.632	1.00	40.11	6
O	ARG	A	3	27.841	-0.823	17.798	1.00	40.63	8
N	ASP	A	3	27.683	1.330	18.381	1.00	39.98	7
CA	ASP	A	3	28.670	1.282	19.440	1.00	40.06	6
CB	ASP	A	3	29.519	2.566	19.359	1.00	39.64	6
C	ASP	A	3	30.451	2.630	18.176	1.00	40.62	6
O	ASP	A	3	30.287	1.857	17.211	1.00	42.45	8
O	ASP	A	3	31.377	3.472	18.203	1.00	42.37	8
C	ASP	A	3	28.094	1.233	20.843	1.00	40.44	6
O	ASP	A	3	28.839	1.293	21.827	1.00	40.41	8
N	GLN	A	3	26.775	1.261	20.977	1.00	40.68	7
CA	GLN	A	3	26.120	1.289	22.279	1.00	41.07	6
CB	GLN	A	3	26.060	-0.110	22.889	1.00	41.34	6
C	GLN	A	3	25.441	-1.157	21.980	1.00	43.02	6
C	GLN	A	3	23.932	-1.101	21.920	1.00	43.88	6
O	GLN	A	3	23.254	-0.919	22.930	1.00	43.71	8
N	GLN	A	3	23.379	-1.258	20.720	1.00	45.09	7
C	GLN	A	3	26.773	2.285	23.235	1.00	40.94	6
O	GLN	A	3	26.900	2.032	24.433	1.00	41.47	8
N	ALA	A	3	26.982	3.509	22.772	1.00	40.54	7
CA	ALA	A	3	27.526	4.607	23.550	1.00	40.25	6
CB	ALA	A	3	29.003	4.811	23.267	1.00	39.67	6
C	ALA	A	3	26.733	5.869	23.207	1.00	40.54	6
O	ALA	A	3	26.398	6.083	22.041	1.00	40.55	8
N	VAL	A	3	26.400	6.655	24.220	1.00	40.29	7
CA	VAL	A	3	25.621	7.873	24.018	1.00	40.33	6
CB	VAL	A	3	24.326	7.849	24.847	1.00	41.69	6
C	VAL	A	3	23.693	9.228	24.973	1.00	44.15	6
C	VAL	A	3	23.316	6.886	24.230	1.00	42.65	6
C	VAL	A	3	26.461	9.099	24.356	1.00	39.55	6
O	VAL	A	3	26.954	9.232	25.472	1.00	39.88	8
N	PRO	A	3	26.593	10.004	23.392	1.00	38.67	7

C	PRO	A	3	25.982	9.912	22.044	1.00	38.43	6
CA	PRO	A	3	27.341	11.232	23.561	1.00	37.39	6
CB	PRO	A	3	27.373	11.879	22.188	1.00	37.81	6
C	PRO	A	3	26.699	10.959	21.245	1.00	38.10	6
C	PRO	A	3	26.636	12.149	24.582	1.00	36.31	6
O	PRO	A	3	25.463	12.195	24.703	1.00	36.61	8
N	PRO	A	3	27.502	12.897	25.314	1.00	34.96	7
C	PRO	A	3	28.985	12.873	25.229	1.00	34.65	6
CA	PRO	A	3	27.030	13.776	26.355	1.00	34.12	6
CB	PRO	A	3	28.269	13.948	27.243	1.00	34.16	6
C	PRO	A	3	29.419	13.827	26.307	1.00	34.54	6
C	PRO	A	3	26.562	15.158	25.945	1.00	33.33	6
O	PRO	A	3	26.823	15.673	24.864	1.00	32.70	8
N	THR	A	3	25.873	15.790	26.892	1.00	33.07	7
CA	THR	A	3	25.505	17.193	26.785	1.00	33.34	6
CB	THR	A	3	24.125	17.525	27.365	1.00	32.36	6
O	THR	A	3	23.125	16.690	26.775	1.00	34.77	8
C	THR	A	3	23.787	18.987	27.116	1.00	30.68	6
C	THR	A	3	26.572	17.928	27.607	1.00	33.64	6
O	THR	A	3	26.393	17.987	28.824	1.00	34.29	8
N	ILE	A	3	27.709	18.280	27.019	1.00	33.67	7
CA	ILE	A	3	28.753	18.913	27.829	1.00	34.08	6
CB	ILE	A	3	30.091	19.062	27.090	1.00	31.83	6
C	ILE	A	3	30.542	17.710	26.551	1.00	31.40	6
C	ILE	A	3	30.011	20.091	25.963	1.00	31.66	6
C	ILE	A	3	31.348	20.624	25.497	1.00	27.91	6
C	ILE	A	3	28.267	20.259	28.343	1.00	34.65	6
O	ILE	A	3	27.273	20.813	27.877	1.00	34.80	8
N	ASN	A	3	28.953	20.806	29.338	1.00	35.52	7
CA	ASN	A	3	28.678	22.085	29.954	1.00	36.17	6
CB	ASN	A	3	28.564	23.192	28.895	1.00	37.53	6
C	ASN	A	3	29.853	23.478	28.157	1.00	39.33	6
O	ASN	A	3	30.942	23.435	28.729	1.00	41.49	8
N	ASN	A	3	29.725	23.759	26.865	1.00	38.26	7
C	ASN	A	3	27.438	22.141	30.834	1.00	37.42	6
O	ASN	A	3	27.059	23.240	31.267	1.00	36.65	8
N	LEU	A	3	26.805	21.021	31.152	1.00	39.20	7
CA	LEU	A	3	25.583	21.032	31.951	1.00	41.87	6
CB	LEU	A	3	24.686	19.861	31.559	1.00	39.97	6
C	LEU	A	3	23.296	19.758	32.183	1.00	39.36	6
C	LEU	A	3	22.575	21.095	32.216	1.00	39.37	6
C	LEU	A	3	22.457	18.727	31.438	1.00	37.75	6
C	LEU	A	3	25.891	21.037	33.443	1.00	44.02	6
O	LEU	A	3	25.739	20.048	34.153	1.00	43.56	8
N	ASP	A	3	26.281	22.205	33.940	1.00	46.66	7
CA	ASP	A	3	26.700	22.407	35.311	1.00	49.49	6
CB	ASP	A	3	27.590	23.656	35.391	1.00	50.43	6
C	ASP	A	3	28.868	23.531	34.591	1.00	50.97	6
O	ASP	A	3	29.356	24.568	34.092	1.00	52.47	8
O	ASP	A	3	29.393	22.406	34.463	1.00	51.53	8
C	ASP	A	3	25.533	22.583	36.271	1.00	51.39	6
O	ASP	A	3	25.652	22.273	37.457	1.00	52.19	8
N	ASN	A	3	24.415	23.097	35.773	1.00	52.98	7
CA	ASN	A	3	23.240	23.333	36.597	1.00	54.38	6
CB	ASN	A	3	23.354	24.718	37.246	1.00	55.67	6
C	ASN	A	3	23.817	24.718	38.683	1.00	56.56	6
O	ASN	A	3	23.364	23.912	39.498	1.00	58.64	8
N	ASN	A	3	24.732	25.628	39.001	1.00	54.49	7
C	ASN	A	3	21.945	23.281	35.796	1.00	55.65	6
O	ASN	A	3	21.533	24.272	35.192	1.00	55.61	8
N	PRO	A	3	21.269	22.139	35.827	1.00	56.99	7
C	PRO	A	3	21.700	20.916	36.544	1.00	56.97	6
CA	PRO	A	3	20.000	21.961	35.149	1.00	58.36	6
CB	PRO	A	3	19.505	20.603	35.633	1.00	57.72	6

Figure 1 - 21

C	PRO	A	3	20.703	19.878	36.120	1.00	57.10	6
C	PRO	A	3	18.996	23.049	35.491	1.00	60.26	6
O	PRO	A	3	19.009	23.592	36.597	1.00	60.43	8
N	ASP	A	3	18.120	23.370	34.544	1.00	62.72	7
CA	ASP	A	3	17.091	24.389	34.766	1.00	65.42	6
CB	ASP	A	3	16.358	24.680	33.461	1.00	65.96	6
C	ASP	A	3	15.930	26.125	33.310	1.00	66.13	6
O	ASP	A	3	16.724	27.026	33.650	1.00	66.02	8
O	ASP	A	3	14.791	26.358	32.850	1.00	66.29	8
C	ASP	A	3	16.146	23.894	35.856	1.00	67.55	6
O	ASP	A	3	16.062	22.683	36.086	1.00	67.61	8
N	GLU	A	3	15.435	24.785	36.534	1.00	69.63	7
CA	GLU	A	3	14.574	24.425	37.650	1.00	71.91	6
CB	GLU	A	3	13.891	25.670	38.236	1.00	75.55	6
C	GLU	A	3	12.875	26.305	37.311	1.00	80.01	6
C	GLU	A	3	11.769	27.059	38.015	1.00	82.31	6
O	GLU	A	3	10.586	26.784	37.716	1.00	83.41	8
O	GLU	A	3	12.072	27.930	38.856	1.00	83.82	8
C	GLU	A	3	13.522	23.369	37.350	1.00	72.78	6
O	GLU	A	3	13.282	22.501	38.198	1.00	73.13	8
N	GLY	A	3	12.857	23.430	36.204	1.00	73.37	7
CA	GLY	A	3	11.854	22.436	35.831	1.00	73.98	6
C	GLY	A	3	12.445	21.469	34.805	1.00	74.22	6
O	GLY	A	3	11.937	21.288	33.703	1.00	74.73	8
N	CYS	A	3	13.556	20.859	35.182	1.00	74.04	7
CA	CYS	A	3	14.279	19.887	34.372	1.00	73.35	6
CB	CYS	A	3	15.607	20.434	33.873	1.00	74.61	6
SG	CYS	A	3	15.467	21.537	32.442	1.00	75.82	1
C	CYS	A	3	14.457	18.656	35.264	1.00	72.43	6
O	CYS	A	3	14.589	18.836	36.482	1.00	72.96	8
N	ASP	A	3	14.240	17.458	34.736	1.00	70.74	7
CA	ASP	A	3	14.193	16.275	35.592	1.00	68.42	6
CB	ASP	A	3	12.750	16.087	36.082	1.00	73.06	6
C	ASP	A	3	12.572	16.349	37.563	1.00	76.10	6
O	ASP	A	3	12.705	17.519	37.983	1.00	77.34	8
O	ASP	A	3	12.283	15.389	38.308	1.00	77.87	8
C	ASP	A	3	14.644	15.011	34.878	1.00	65.39	6
O	ASP	A	3	14.655	13.929	35.468	1.00	65.66	8
N	LEU	A	3	14.976	15.137	33.600	1.00	61.63	7
CA	LEU	A	3	15.371	13.988	32.798	1.00	57.08	6
CB	LEU	A	3	14.923	14.189	31.345	1.00	55.81	6
C	LEU	A	3	13.488	14.681	31.137	1.00	54.21	6
C	LEU	A	3	13.376	15.503	29.863	1.00	53.80	6
C	LEU	A	3	12.523	13.506	31.107	1.00	53.91	6
C	LEU	A	3	16.876	13.755	32.832	1.00	53.93	6
O	LEU	A	3	17.651	14.633	33.214	1.00	53.81	8
N	ASP	A	3	17.279	12.559	32.412	1.00	50.75	7
CA	ASP	A	3	18.700	12.234	32.329	1.00	47.57	6
CB	ASP	A	3	18.957	10.737	32.446	1.00	47.56	6
C	ASP	A	3	20.434	10.393	32.426	1.00	47.70	6
O	ASP	A	3	20.789	9.300	31.938	1.00	48.81	8
O	ASP	A	3	21.250	11.214	32.895	1.00	48.47	8
C	ASP	A	3	19.226	12.766	30.995	1.00	45.22	6
O	ASP	A	3	19.021	12.170	29.939	1.00	43.88	8
N	PHE	A	3	19.926	13.893	31.053	1.00	43.38	7
CA	PHE	A	3	20.451	14.559	29.873	1.00	42.15	6
CB	PHE	A	3	20.418	16.078	30.088	1.00	41.31	6
C	PHE	A	3	19.057	16.688	30.234	1.00	42.33	6
C	PHE	A	3	18.735	17.421	31.366	1.00	42.04	6
C	PHE	A	3	18.092	16.544	29.250	1.00	42.50	6
CE	PHE	A	3	17.486	17.992	31.515	1.00	41.44	6
CE	PHE	A	3	16.842	17.111	29.391	1.00	42.67	6
CZ	PHE	A	3	16.538	17.837	30.526	1.00	42.42	6
C	PHE	A	3	21.871	14.141	29.516	1.00	41.29	6

O	PHE	A	3	22.597	14.874	28.844	1.00	40.83	8
N	VAL	A	3	22.307	12.972	29.970	1.00	40.72	7
CA	VAL	A	3	23.650	12.448	29.776	1.00	40.16	6
CB	VAL	A	3	23.891	11.815	28.403	1.00	38.09	6
C	VAL	A	3	25.173	10.990	28.427	1.00	36.99	6
C	VAL	A	3	22.727	10.932	27.974	1.00	38.10	6
C	VAL	A	3	24.659	13.563	30.056	1.00	40.38	6
O	VAL	A	3	25.385	14.035	29.186	1.00	40.38	8
N	PRO	A	3	24.700	14.009	31.313	1.00	40.78	7
C	PRO	A	3	23.800	13.524	32.404	1.00	40.85	6
CA	PRO	A	3	25.309	15.254	31.696	1.00	40.90	6
CB	PRO	A	3	25.114	15.342	33.216	1.00	40.96	6
C	PRO	A	3	24.428	14.100	33.638	1.00	40.79	6
C	PRO	A	3	26.734	15.593	31.358	1.00	41.19	6
O	PRO	A	3	26.904	16.768	30.971	1.00	42.24	8
N	HIS	A	3	27.780	14.807	31.590	1.00	40.96	7
CA	HIS	A	3	29.125	15.321	31.308	1.00	40.86	6
CB	HIS	A	3	29.855	15.671	32.615	1.00	40.66	6
C	HIS	A	3	29.399	16.966	33.216	1.00	40.73	6
C	HIS	A	3	29.717	18.252	32.951	1.00	41.56	6
N	HIS	A	3	28.427	17.004	34.194	1.00	41.70	7
CE	HIS	A	3	28.196	18.257	34.535	1.00	40.82	6
N	HIS	A	3	28.964	19.035	33.793	1.00	42.13	7
C	HIS	A	3	29.998	14.402	30.476	1.00	40.86	6
O	HIS	A	3	30.871	14.875	29.743	1.00	39.80	8
N	GLU	A	3	29.799	13.098	30.610	1.00	41.82	7
CA	GLU	A	3	30.603	12.134	29.866	1.00	42.65	6
CB	GLU	A	3	31.560	11.395	30.800	1.00	48.00	6
C	GLU	A	3	33.025	11.769	30.651	1.00	54.38	6
C	GLU	A	3	33.949	10.601	30.938	1.00	58.70	6
O	GLU	A	3	34.307	10.398	32.118	1.00	62.14	8
O	GLU	A	3	34.320	9.878	29.990	1.00	60.16	8
C	GLU	A	3	29.690	11.143	29.152	1.00	41.91	6
O	GLU	A	3	28.533	10.976	29.536	1.00	41.07	8
N	ALA	A	3	30.220	10.524	28.105	1.00	41.81	7
CA	ALA	A	3	29.453	9.543	27.348	1.00	41.61	6
CB	ALA	A	3	30.301	8.960	26.230	1.00	41.62	6
C	ALA	A	3	28.964	8.436	28.276	1.00	41.80	6
O	ALA	A	3	29.691	8.012	29.176	1.00	41.92	8
N	ARG	A	3	27.726	7.999	28.069	1.00	41.60	7
CA	ARG	A	3	27.181	6.905	28.866	1.00	40.84	6
CB	ARG	A	3	25.735	7.170	29.277	1.00	40.27	6
C	ARG	A	3	25.176	6.134	30.241	1.00	39.78	6
C	ARG	A	3	25.303	6.599	31.683	1.00	38.06	6
N	ARG	A	3	24.282	7.589	32.015	1.00	38.84	7
CZ	ARG	A	3	24.534	8.880	32.190	1.00	41.57	6
N	ARG	A	3	25.771	9.349	32.071	1.00	43.04	7
N	ARG	A	3	23.545	9.711	32.490	1.00	42.78	7
C	ARG	A	3	27.280	5.603	28.078	1.00	40.36	6
O	ARG	A	3	27.220	5.612	26.850	1.00	40.45	8
N	GLN	A	3	27.494	4.502	28.783	1.00	40.51	7
CA	GLN	A	3	27.539	3.181	28.159	1.00	39.98	6
CB	GLN	A	3	28.581	2.309	28.851	1.00	41.17	6
C	GLN	A	3	28.564	0.840	28.470	1.00	42.05	6
C	GLN	A	3	29.364	0.558	27.216	1.00	41.53	6
O	GLN	A	3	28.850	-0.009	26.251	1.00	44.79	8
N	GLN	A	3	30.629	0.959	27.223	1.00	40.43	7
C	GLN	A	3	26.151	2.558	28.260	1.00	39.51	6
O	GLN	A	3	25.491	2.744	29.287	1.00	39.97	8
N	VAL	A	3	25.644	1.971	27.185	1.00	39.03	7
CA	VAL	A	3	24.332	1.327	27.199	1.00	38.60	6
CB	VAL	A	3	23.234	2.055	26.417	1.00	37.27	6
C	VAL	A	3	22.917	3.429	27.001	1.00	37.12	6
C	VAL	A	3	23.579	2.190	24.942	1.00	34.97	6

Figure 1 - 22

C	VAL	A	3	24.491	-0.100	26.668	1.00	38.94	6
O	VAL	A	3	25.540	-0.387	26.081	1.00	38.81	8
N	SER	A	3	23.501	-0.967	26.865	1.00	39.38	7
CA	SER	A	3	23.663	-2.356	26.464	1.00	40.73	6
CB	SER	A	3	23.649	-3.252	27.720	1.00	40.55	6
O	SER	A	3	23.861	-4.601	27.327	1.00	42.48	8
C	SER	A	3	22.681	-2.919	25.456	1.00	41.20	6
O	SER	A	3	23.144	-3.476	24.447	1.00	41.74	8
N	GLY	A	3	21.377	-2.851	25.686	1.00	41.13	7
CA	GLY	A	3	20.429	-3.435	24.741	1.00	42.12	6
C	GLY	A	3	19.550	-2.401	24.054	1.00	42.75	6
O	GLY	A	3	18.326	-2.538	24.022	1.00	42.94	8
N	MET	A	3	20.167	-1.367	23.500	1.00	43.16	7
CA	MET	A	3	19.440	-0.299	22.822	1.00	43.71	6
CB	MET	A	3	20.230	1.004	22.944	1.00	43.69	6
C	MET	A	3	19.642	2.207	22.232	1.00	43.01	6
SD	MET	A	3	20.366	3.767	22.774	1.00	43.68	1
CE	MET	A	3	21.976	3.688	21.993	1.00	42.01	6
C	MET	A	3	19.192	-0.651	21.361	1.00	44.30	6
O	MET	A	3	20.141	-0.930	20.627	1.00	44.01	8
N	GLU	A	3	17.931	-0.626	20.941	1.00	45.44	7
CA	GLU	A	3	17.587	-0.949	19.560	1.00	46.71	6
CB	GLU	A	3	16.583	-2.106	19.526	1.00	52.33	6
C	GLU	A	3	16.984	-3.255	18.615	1.00	57.87	6
C	GLU	A	3	16.009	-4.416	18.694	1.00	61.10	6
O	GLU	A	3	16.263	-5.350	19.485	1.00	63.46	8
O	GLU	A	3	14.991	-4.392	17.973	1.00	61.67	8
C	GLU	A	3	17.025	0.239	18.789	1.00	46.35	6
O	GLU	A	3	17.177	0.304	17.565	1.00	46.24	8
N	TYR	A	3	16.373	1.173	19.474	1.00	45.47	7
CA	TYR	A	3	15.785	2.334	18.820	1.00	44.72	6
CB	TYR	A	3	14.269	2.389	19.063	1.00	45.79	6
C	TYR	A	3	13.494	1.272	18.401	1.00	47.57	6
C	TYR	A	3	13.104	0.157	19.132	1.00	48.71	6
CE	TYR	A	3	12.420	-0.886	18.535	1.00	49.56	6
C	TYR	A	3	13.182	1.313	17.051	1.00	48.28	6
CE	TYR	A	3	12.496	0.277	16.445	1.00	49.38	6
CZ	TYR	A	3	12.119	-0.819	17.192	1.00	50.16	6
O	TYR	A	3	11.437	-1.855	16.597	1.00	51.10	8
C	TYR	A	3	16.390	3.650	19.294	1.00	43.38	6
O	TYR	A	3	16.662	3.827	20.482	1.00	43.12	8
N	THR	A	3	16.541	4.606	18.381	1.00	41.59	7
CA	THR	A	3	16.920	5.968	18.718	1.00	39.98	6
CB	THR	A	3	18.373	6.345	18.388	1.00	40.58	6
O	THR	A	3	18.696	5.961	17.044	1.00	38.16	8
C	THR	A	3	19.360	5.709	19.354	1.00	41.15	6
C	THR	A	3	16.008	6.965	17.995	1.00	38.98	6
O	THR	A	3	15.540	6.724	16.887	1.00	38.49	8
N	LEU	A	3	15.788	8.107	18.626	1.00	38.40	7
CA	LEU	A	3	14.951	9.179	18.101	1.00	37.48	6
CB	LEU	A	3	13.862	9.461	19.134	1.00	40.89	6
C	LEU	A	3	12.706	10.398	18.820	1.00	43.96	6
C	LEU	A	3	11.655	9.721	17.955	1.00	45.59	6
C	LEU	A	3	12.058	10.894	20.110	1.00	45.23	6
C	LEU	A	3	15.778	10.431	17.835	1.00	36.55	6
O	LEU	A	3	16.477	10.888	18.745	1.00	36.35	8
N	CYS	A	3	15.754	10.970	16.616	1.00	35.33	7
CA	CYS	A	3	16.465	12.209	16.319	1.00	34.09	6
CB	CYS	A	3	17.441	12.103	15.146	1.00	30.99	6
SG	CYS	A	3	18.186	13.714	14.750	1.00	29.61	1
C	CYS	A	3	15.483	13.347	16.038	1.00	33.67	6
O	CYS	A	3	14.700	13.305	15.093	1.00	34.22	8
N	ASN	A	3	15.558	14.388	16.852	1.00	33.84	7
CA	ASN	A	3	14.661	15.523	16.801	1.00	33.60	6

CB	ASN	A	3	14.226	15.790	18.260	1.00	36.16	6
C	ASN	A	3	13.048	14.951	18.697	1.00	39.16	6
O	ASN	A	3	12.375	14.313	17.887	1.00	41.53	8
N	ASN	A	3	12.774	14.966	19.997	1.00	39.24	7
C	ASN	A	3	15.191	16.827	16.233	1.00	32.97	6
O	ASN	A	3	16.246	17.325	16.617	1.00	32.75	8
N	SER	A	3	14.373	17.483	15.413	1.00	32.66	7
CA	SER	A	3	14.676	18.793	14.851	1.00	31.74	6
CB	SER	A	3	15.200	18.682	13.422	1.00	31.39	6
O	SER	A	3	16.598	18.874	13.359	1.00	31.26	8
C	SER	A	3	13.416	19.656	14.860	1.00	31.57	6
O	SER	A	3	12.435	19.319	14.194	1.00	31.75	8
N	PHE	A	3	13.415	20.722	15.649	1.00	30.83	7
CA	PHE	A	3	12.270	21.619	15.761	1.00	31.51	6
CB	PHE	A	3	11.712	21.643	17.185	1.00	31.46	6
C	PHE	A	3	11.529	20.317	17.862	1.00	32.87	6
C	PHE	A	3	12.125	20.065	19.087	1.00	33.75	6
C	PHE	A	3	10.774	19.310	17.280	1.00	33.53	6
CE	PHE	A	3	11.976	18.843	19.714	1.00	33.89	6
CE	PHE	A	3	10.633	18.082	17.894	1.00	35.78	6
CZ	PHE	A	3	11.227	17.850	19.119	1.00	33.73	6
C	PHE	A	3	12.688	23.029	15.347	1.00	31.43	6
O	PHE	A	3	13.279	23.753	16.150	1.00	31.64	8
N	GLY	A	3	12.398	23.442	14.116	1.00	31.34	7
CA	GLY	A	3	12.972	24.648	13.571	1.00	30.81	6
C	GLY	A	3	12.146	25.906	13.465	1.00	30.77	6
O	GLY	A	3	10.939	25.956	13.680	1.00	29.83	8
N	PHE	A	4	12.847	26.982	13.095	1.00	31.24	7
CA	PHE	A	4	12.239	28.297	12.897	1.00	31.72	6
CB	PHE	A	4	13.280	29.283	12.373	1.00	35.13	6
C	PHE	A	4	14.430	29.453	13.330	1.00	37.25	6
C	PHE	A	4	15.692	28.998	13.002	1.00	39.09	6
C	PHE	A	4	14.245	30.067	14.558	1.00	38.34	6
CE	PHE	A	4	16.752	29.147	13.876	1.00	38.52	6
CE	PHE	A	4	15.299	30.220	15.436	1.00	38.09	6
CZ	PHE	A	4	16.555	29.759	15.095	1.00	37.29	6
C	PHE	A	4	11.042	28.155	11.971	1.00	30.64	6
O	PHE	A	4	11.052	27.334	11.054	1.00	30.82	8
N	GLY	A	4	9.976	28.894	12.261	1.00	29.80	7
CA	GLY	A	4	8.742	28.810	11.489	1.00	28.76	6
C	GLY	A	4	7.805	27.760	12.082	1.00	27.97	6
O	GLY	A	4	6.727	27.488	11.554	1.00	28.67	8
N	GLY	A	4	8.217	27.113	13.162	1.00	26.86	7
CA	GLY	A	4	7.475	26.074	13.835	1.00	26.12	6
C	GLY	A	4	7.370	24.786	13.036	1.00	26.70	6
O	GLY	A	4	6.376	24.071	13.171	1.00	27.71	8
N	THR	A	4	8.377	24.450	12.237	1.00	25.43	7
CA	THR	A	4	8.323	23.222	11.440	1.00	24.02	6
CB	THR	A	4	8.749	23.499	9.993	1.00	21.80	6
O	THR	A	4	8.766	22.279	9.243	1.00	19.29	8
C	THR	A	4	10.113	24.167	9.915	1.00	20.36	6
C	THR	A	4	9.131	22.138	12.134	1.00	24.60	6
O	THR	A	4	10.324	22.291	12.401	1.00	24.92	8
N	ASN	A	4	8.455	21.061	12.542	1.00	24.70	7
CA	ASN	A	4	9.067	20.005	13.322	1.00	24.60	6
CB	ASN	A	4	8.250	19.701	14.591	1.00	23.50	6
C	ASN	A	4	7.907	20.924	15.404	1.00	23.01	6
O	ASN	A	4	8.801	21.625	15.878	1.00	26.17	8
N	ASN	A	4	6.616	21.179	15.556	1.00	22.16	7
C	ASN	A	4	9.204	18.667	12.604	1.00	24.49	6
O	ASN	A	4	8.407	18.309	11.745	1.00	24.10	8
N	GLY	A	4	10.187	17.896	13.071	1.00	24.98	7
CA	GLY	A	4	10.420	16.572	12.516	1.00	26.39	6
C	GLY	A	4	11.169	15.675	13.491	1.00	26.58	6

Figure 1 - 23

N	ARG	B	4	-11.838	10.004	-7.911	0.00	0.00	7
C	ARG	B	4	-6.886	11.333	-3.435	0.00	0.00	6
O	ARG	B	4	-7.460	11.712	-2.416	0.00	0.00	8
N	VAL	B	5	-6.150	12.141	-4.194	0.00	0.00	7
CA	VAL	B	5	-5.980	13.555	-3.891	0.00	0.00	6
CB	VAL	B	5	-4.499	13.967	-3.796	0.00	0.00	6
C	VAL	B	5	-4.375	15.410	-3.320	0.00	0.00	6
C	VAL	B	5	-3.712	13.046	-2.877	0.00	0.00	6
C	VAL	B	5	-6.649	14.423	-4.953	0.00	0.00	6
O	VAL	B	5	-6.439	14.236	-6.151	0.00	0.00	8
N	VAL	B	6	-7.458	15.377	-4.506	0.00	0.00	7
CA	VAL	B	6	-8.162	16.289	-5.394	0.00	0.00	6
CB	VAL	B	6	-9.689	16.096	-5.351	0.00	0.00	6
C	VAL	B	6	-10.108	14.791	-6.013	0.00	0.00	6
C	VAL	B	6	-10.207	16.146	-3.921	0.00	0.00	6
C	VAL	B	6	-7.835	17.739	-5.044	0.00	0.00	6
O	VAL	B	6	-7.351	18.031	-3.954	0.00	0.00	8
N	VAL	B	7	-8.082	18.647	-5.981	0.00	0.00	7
CA	VAL	B	7	-7.829	20.072	-5.781	0.00	0.00	6
CB	VAL	B	7	-7.171	20.707	-7.016	0.00	0.00	6
C	VAL	B	7	-6.746	22.142	-6.786	0.00	0.00	6
C	VAL	B	7	-5.973	19.884	-7.474	0.00	0.00	6
C	VAL	B	7	-9.141	20.780	-5.464	0.00	0.00	6
O	VAL	B	7	-10.056	20.800	-6.287	0.00	0.00	8
N	THR	B	8	-9.248	21.344	-4.264	0.00	0.00	7
CA	THR	B	8	-10.464	22.008	-3.833	0.00	0.00	6
CB	THR	B	8	-10.960	21.391	-2.496	0.00	0.00	6
O	THR	B	8	-10.012	21.721	-1.470	0.00	0.00	8
C	THR	B	8	-11.126	19.888	-2.579	0.00	0.00	6
C	THR	B	8	-10.367	23.504	-3.600	0.00	0.00	6
O	THR	B	8	-11.293	24.068	-3.004	0.00	0.00	8
N	GLY	B	9	-9.286	24.153	-4.005	0.00	0.00	7
CA	GLY	B	9	-9.144	25.589	-3.757	0.00	0.00	6
C	GLY	B	9	-7.950	26.136	-4.528	0.00	0.00	6
O	GLY	B	9	-6.886	25.518	-4.564	0.00	0.00	8
N	LEU	B	1	-8.152	27.280	-5.174	0.00	0.00	7
CA	LEU	B	1	-7.105	27.900	-5.976	0.00	0.00	6
CB	LEU	B	1	-7.446	27.838	-7.465	0.00	0.00	6
C	LEU	B	1	-7.764	26.482	-8.091	0.00	0.00	6
C	LEU	B	1	-8.238	26.644	-9.528	0.00	0.00	6
C	LEU	B	1	-6.558	25.554	-8.027	0.00	0.00	6
C	LEU	B	1	-6.897	29.350	-5.557	0.00	0.00	6
O	LEU	B	1	-7.841	30.024	-5.142	0.00	0.00	8
N	GLY	B	1	-5.664	29.823	-5.668	0.00	0.00	7
CA	GLY	B	1	-5.349	31.207	-5.306	0.00	0.00	6
C	GLY	B	1	-4.062	31.628	-6.007	0.00	0.00	6
O	GLY	B	1	-3.216	30.774	-6.284	0.00	0.00	8
N	MET	B	1	-3.931	32.914	-6.317	0.00	0.00	7
CA	MET	B	1	-2.727	33.388	-6.974	0.00	0.00	6
CB	MET	B	1	-2.490	32.625	-8.282	0.00	0.00	6
C									

CA	SER	B	1	0.573	37.004	-11.205	0.00	0.00	6
CB	SER	B	1	-0.015	35.962	-12.155	0.00	0.00	6
O	SER	B	1	-0.875	36.553	-13.112	0.00	0.00	8
C	SER	B	1	0.707	38.350	-11.895	0.00	0.00	6
O	SER	B	1	-0.036	39.287	-11.612	0.00	0.00	8
N	PRO	B	1	1.592	38.431	-12.880	0.00	0.00	7
C	PRO	B	1	2.528	37.351	-13.288	0.00	0.00	6
CA	PRO	B	1	1.796	39.632	-13.665	0.00	0.00	6
CB	PRO	B	1	3.008	39.317	-14.535	0.00	0.00	6
C	PRO	B	1	3.661	38.139	-13.902	0.00	0.00	6
C	PRO	B	1	0.602	40.043	-14.509	0.00	0.00	6
O	PRO	B	1	0.561	41.209	-14.924	0.00	0.00	8
N	VAL	B	1	-0.355	39.168	-14.817	0.00	0.00	7
CA	VAL	B	1	-1.521	39.561	-15.592	0.00	0.00	6
CB	VAL	B	1	-1.781	38.692	-16.836	0.00	0.00	6
C	VAL	B	1	-0.708	38.926	-17.890	0.00	0.00	6
C	VAL	B	1	-1.882	37.219	-16.477	0.00	0.00	6
C	VAL	B	1	-2.799	39.600	-14.761	0.00	0.00	6
O	VAL	B	1	-3.883	39.725	-15.340	0.00	0.00	8
N	GLY	B	1	-2.703	39.502	-13.440	0.00	0.00	7
CA	GLY	B	1	-3.904	39.542	-12.612	0.00	0.00	6
C	GLY	B	1	-3.619	39.258	-11.146	0.00	0.00	6
O	GLY	B	1	-2.708	38.499	-10.817	0.00	0.00	8
N	ASN	B	1	-4.419	39.856	-10.269	0.00	0.00	7
CA	ASN	B	1	-4.271	39.693	-8.833	0.00	0.00	6
CB	ASN	B	1	-4.557	41.013	-8.113	0.00	0.00	6
C	ASN	B	1	-3.346	41.910	-7.977	0.00	0.00	6
O	ASN	B	1	-2.706	42.284	-8.961	0.00	0.00	8
N	ASN	B	1	-3.014	42.291	-6.748	0.00	0.00	7
C	ASN	B	1	-5.170	38.603	-8.269	0.00	0.00	6
O	ASN	B	1	-5.198	38.386	-7.058	0.00	0.00	8
N	THR	B	1	-5.984	37.976	-9.104	0.00	0.00	7
CA	THR	B	1	-6.834	36.866	-8.721	0.00	0.00	6
CB	THR	B	1	-8.337	37.195	-8.653	0.00	0.00	6
O	THR	B	1	-8.753	37.727	-9.920	0.00	0.00	8
C	THR	B	1	-8.673	38.174	-7.548	0.00	0.00	6
C	THR	B	1	-6.685	35.733	-9.743	0.00	0.00	6
O	THR	B	1	-6.175	35.946	-10.840	0.00	0.00	8
N	VAL	B	2	-7.245	34.576	-9.417	0.00	0.00	7
CA	VAL	B	2	-7.206	33.430	-10.309	0.00	0.00	6
CB	VAL	B	2	-7.775	32.172	-9.621	0.00	0.00	6
C	VAL	B	2	-7.815	30.979	-10.564	0.00	0.00	6
C	VAL	B	2	-6.945	31.826	-8.392	0.00	0.00	6
C	VAL	B	2	-7.959	33.676	-11.609	0.00	0.00	6
O	VAL	B	2	-7.390	33.528	-12.694	0.00	0.00	8
N	GLU	B	2	-9.235	34.032	-11.517	0.00	0.00	7
CA	GLU	B	2	-10.064	34.260	-12.692	0.00	0.00	6
CB	GLU	B	2	-11.531	34.440	-12.281	0.00	0.00	6
C	GLU	B	2	-12.137	33.233	-11.590	0.00	0.00	6
C	GLU	B	2	-12.288	32.006	-12.464	0.00	0.00	6
O	GLU	B	2	-12.184	32.123	-13.703	0.00	0.00	8
O	GLU	B	2	-12.522	30.903	-11.919	0.00	0.00	8
C	GLU	B	2	-9.599	35.406	-13.571	0.00	0.00	6
O	GLU	B	2	-9.489	35.218	-14.789	0.00	0.00	8
N	SER	B	2	-9.214	36.545	-13.005	0.00	0.00	7
CA	SER	B	2	-8.706	37.658	-13.805	0.00	0.00	6
CB	SER	B	2	-8.514	38.913	-12.967	0.00	0.00	6
O	SER	B	2	-7.593	38.724	-11.911	0.00	0.00	8
C	SER	B	2	-7.429	37.252	-14.529	0.00	0.00	6
O	SER	B	2	-7.234	37.591	-15.698	0.00	0.00	8
N	THR	B	2	-6.555	36.509	-13.854	0.00	0.00	7
CA	THR	B	2	-5.319	36.021	-14.459	0.00	0.00	6
CB	THR	B	2	-4.442	35.270	-13.444	0.00	0.00	6
O	THR	B	2	-3.761	36.220	-12.614	0.00	0.00	8

Figure 1 - 25

C	THR	B	2	-3.400	34.381	-14.101	0.00	0.00	6
C	THR	B	2	-5.685	35.070	-15.601	0.00	0.00	6
O	THR	B	2	-5.100	35.126	-16.681	0.00	0.00	8
N	TRP	B	2	-6.625	34.166	-15.337	0.00	0.00	7
CA	TRP	B	2	-7.069	33.187	-16.324	0.00	0.00	6
CB	TRP	B	2	-8.124	32.257	-15.721	0.00	0.00	6
C	TRP	B	2	-8.554	31.131	-16.610	0.00	0.00	6
C	TRP	B	2	-7.715	30.225	-17.335	0.00	0.00	6
CE	TRP	B	2	-8.556	29.338	-18.035	0.00	0.00	6
CE	TRP	B	2	-6.330	30.079	-17.462	0.00	0.00	6
C	TRP	B	2	-9.839	30.763	-16.892	0.00	0.00	6
N	TRP	B	2	-9.849	29.686	-17.746	0.00	0.00	7
CZ	TRP	B	2	-8.062	28.322	-18.849	0.00	0.00	6
CZ	TRP	B	2	-5.840	29.069	-18.269	0.00	0.00	6
C	TRP	B	2	-6.704	28.201	-18.952	0.00	0.00	6
C	TRP	B	2	-7.583	33.858	-17.592	0.00	0.00	6
O	TRP	B	2	-7.160	33.508	-18.694	0.00	0.00	8
N	LYS	B	2	-8.470	34.834	-17.456	0.00	0.00	7
CA	LYS	B	2	-9.042	35.564	-18.576	0.00	0.00	6
CB	LYS	B	2	-10.109	36.555	-18.097	0.00	0.00	6
C	LYS	B	2	-11.283	35.913	-17.377	0.00	0.00	6
C	LYS	B	2	-12.370	36.937	-17.083	0.00	0.00	6
CE	LYS	B	2	-13.606	36.274	-16.497	0.00	0.00	6
NZ	LYS	B	2	-14.851	36.738	-17.170	0.00	0.00	7
C	LYS	B	2	-8.001	36.320	-19.393	0.00	0.00	6
O	LYS	B	2	-8.069	36.331	-20.626	0.00	0.00	8
N	ALA	B	2	-7.024	36.927	-18.727	0.00	0.00	7
CA	ALA	B	2	-5.956	37.637	-19.422	0.00	0.00	6
CB	ALA	B	2	-5.089	38.401	-18.433	0.00	0.00	6
C	ALA	B	2	-5.117	36.686	-20.267	0.00	0.00	6
O	ALA	B	2	-4.735	37.026	-21.390	0.00	0.00	8
N	LEU	B	2	-4.852	35.485	-19.765	0.00	0.00	7
CA	LEU	B	2	-4.074	34.491	-20.487	0.00	0.00	6
CB	LEU	B	2	-3.722	33.310	-19.585	0.00	0.00	6
C	LEU	B	2	-2.629	33.472	-18.534	0.00	0.00	6
C	LEU	B	2	-2.164	32.095	-18.065	0.00	0.00	6
C	LEU	B	2	-1.441	34.278	-19.038	0.00	0.00	6
C	LEU	B	2	-4.782	33.983	-21.736	0.00	0.00	6
O	LEU	B	2	-4.157	33.830	-22.788	0.00	0.00	8
N	LEU	B	2	-6.090	33.756	-21.655	0.00	0.00	7
CA	LEU	B	2	-6.862	33.296	-22.804	0.00	0.00	6
CB	LEU	B	2	-8.251	32.826	-22.371	0.00	0.00	6
C	LEU	B	2	-8.328	31.592	-21.467	0.00	0.00	6
C	LEU	B	2	-9.775	31.260	-21.133	0.00	0.00	6
C	LEU	B	2	-7.647	30.388	-22.099	0.00	0.00	6
C	LEU	B	2	-6.965	34.357	-23.891	0.00	0.00	6
O	LEU	B	2	-6.998	34.023	-25.078	0.00	0.00	8
N	ALA	B	2	-6.884	35.636	-23.540	0.00	0.00	7
CA	ALA	B	2	-6.886	36.733				

O	GLN	B	3	-0.765	38.310	-21.429	0.00	0.00	8
N	SER	B	3	-0.062	40.251	-22.307	0.00	0.00	7
CA	SER	B	3	1.278	40.169	-21.739	0.00	0.00	6
CB	SER	B	3	2.294	40.807	-22.679	0.00	0.00	6
O	SER	B	3	3.597	40.831	-22.140	0.00	0.00	8
C	SER	B	3	1.274	40.874	-20.386	0.00	0.00	6
O	SER	B	3	0.498	41.811	-20.191	0.00	0.00	8
N	GLY	B	3	2.110	40.424	-19.459	0.00	0.00	7
CA	GLY	B	3	2.170	41.044	-18.135	0.00	0.00	6
C	GLY	B	3	3.536	41.687	-17.921	0.00	0.00	6
O	GLY	B	3	3.897	42.130	-16.835	0.00	0.00	8
N	ILE	B	3	4.303	41.749	-19.000	0.00	0.00	7
CA	ILE	B	3	5.671	42.238	-18.997	0.00	0.00	6
CB	ILE	B	3	6.473	41.482	-20.089	0.00	0.00	6
C	ILE	B	3	7.954	41.783	-19.950	0.00	0.00	6
C	ILE	B	3	6.125	40.003	-19.990	0.00	0.00	6
C	ILE	B	3	7.148	38.944	-20.253	0.00	0.00	6
C	ILE	B	3	5.778	43.741	-19.184	0.00	0.00	6
O	ILE	B	3	5.345	44.318	-20.180	0.00	0.00	8
N	SER	B	3	6.393	44.396	-18.204	0.00	0.00	7
CA	SER	B	3	6.552	45.837	-18.154	0.00	0.00	6
CB	SER	B	3	5.698	46.401	-17.008	0.00	0.00	6
O	SER	B	3	4.422	46.810	-17.454	0.00	0.00	8
C	SER	B	3	7.998	46.253	-17.896	0.00	0.00	6
O	SER	B	3	8.837	45.419	-17.558	0.00	0.00	8
N	LEU	B	3	8.270	47.548	-18.011	0.00	0.00	7
CA	LEU	B	3	9.597	48.088	-17.731	0.00	0.00	6
CB	LEU	B	3	9.788	49.454	-18.383	0.00	0.00	6
C	LEU	B	3	10.093	49.512	-19.878	0.00	0.00	6
C	LEU	B	3	10.049	50.952	-20.370	0.00	0.00	6
C	LEU	B	3	11.445	48.888	-20.193	0.00	0.00	6
C	LEU	B	3	9.778	48.224	-16.219	0.00	0.00	6
O	LEU	B	3	8.828	48.607	-15.534	0.00	0.00	8
N	ILE	B	3	10.960	47.910	-15.704	0.00	0.00	7
CA	ILE	B	3	11.197	48.024	-14.264	0.00	0.00	6
CB	ILE	B	3	12.471	47.285	-13.832	0.00	0.00	6
C	ILE	B	3	12.855	47.610	-12.395	0.00	0.00	6
C	ILE	B	3	12.293	45.770	-13.991	0.00	0.00	6
C	ILE	B	3	13.596	45.010	-14.122	0.00	0.00	6
C	ILE	B	3	11.289	49.497	-13.874	0.00	0.00	6
O	ILE	B	3	11.972	50.271	-14.546	0.00	0.00	8
N	ASP	B	3	10.643	49.871	-12.772	0.00	0.00	7
CA	ASP	B	3	10.675	51.259	-12.331	0.00	0.00	6
CB	ASP	B	3	9.336	51.943	-12.629	0.00	0.00	6
C	ASP	B	3	8.143	51.205	-12.064	0.00	0.00	6
O	ASP	B	3	7.473	51.744	-11.160	0.00	0.00	8
O	ASP	B	3	7.855	50.079	-12.525	0.00	0.00	8
C	ASP	B	3	11.031	51.429	-10.863	0.00	0.00	6
O	ASP	B	3	11.153	52.575	-10.414	0.00	0.00	8
N	HIS	B	3	11.266	50.348	-10.127	0.00	0.00	7
CA	HIS	B	3	11.539	50.473	-8.696	0.00	0.00	6
CB	HIS	B	3	10.808	49.400	-7.893	0.00	0.00	6
C	HIS	B	3	11.110	48.005	-8.342	0.00	0.00	6
C	HIS	B	3	10.636	47.274	-9.377	0.00	0.00	6
N	HIS	B	3	12.022	47.210	-7.684	0.00	0.00	7
CE	HIS	B	3	12.091	46.042	-8.295	0.00	0.00	6
N	HIS	B	3	11.264	46.052	-9.324	0.00	0.00	7
C	HIS	B	3	13.020	50.517	-8.359	0.00	0.00	6
O	HIS	B	3	13.389	50.654	-7.190	0.00	0.00	8
N	PHE	B	4	13.883	50.454	-9.362	0.00	0.00	7
CA	PHE	B	4	15.318	50.638	-9.192	0.00	0.00	6
CB	PHE	B	4	16.061	49.447	-8.633	0.00	0.00	6
C	PHE	B	4	16.131	48.199	-9.458	0.00	0.00	6
C	PHE	B	4	15.223	47.174	-9.253	0.00	0.00	6

Figure 1 - 26

C	PHE	B	4	17.120	48.028	-10.416	0.00	0.00	6
CE	PHE	B	4	15.281	46.015	-10.000	0.00	0.00	6
CE	PHE	B	4	17.184	46.867	-11.163	0.00	0.00	6
CZ	PHE	B	4	16.264	45.859	-10.957	0.00	0.00	6
C	PHE	B	4	15.893	51.121	-10.527	0.00	0.00	6
O	PHE	B	4	15.265	50.943	-11.571	0.00	0.00	8
N	ASP	B	4	17.003	51.846	-10.472	0.00	0.00	7
CA	ASP	B	4	17.611	52.372	-11.690	0.00	0.00	6
CB	ASP	B	4	18.687	53.406	-11.349	0.00	0.00	6
C	ASP	B	4	18.923	54.376	-12.491	0.00	0.00	6
O	ASP	B	4	17.932	54.804	-13.121	0.00	0.00	8
O	ASP	B	4	20.095	54.711	-12.759	0.00	0.00	8
C	ASP	B	4	18.201	51.255	-12.541	0.00	0.00	6
O	ASP	B	4	19.158	50.593	-12.140	0.00	0.00	8
N	THR	B	4	17.644	51.053	-13.732	0.00	0.00	7
CA	THR	B	4	18.114	50.015	-14.639	0.00	0.00	6
CB	THR	B	4	16.921	49.251	-15.254	0.00	0.00	6
O	THR	B	4	16.088	50.174	-15.962	0.00	0.00	8
C	THR	B	4	16.100	48.566	-14.175	0.00	0.00	6
C	THR	B	4	19.000	50.539	-15.760	0.00	0.00	6
O	THR	B	4	19.202	49.864	-16.774	0.00	0.00	8
N	SER	B	4	19.645	51.679	-15.568	0.00	0.00	7
CA	SER	B	4	20.508	52.311	-16.548	0.00	0.00	6
CB	SER	B	4	21.084	53.616	-15.972	0.00	0.00	6
O	SER	B	4	20.143	54.668	-16.102	0.00	0.00	8
C	SER	B	4	21.666	51.451	-17.029	0.00	0.00	6
O	SER	B	4	21.952	51.395	-18.226	0.00	0.00	8
N	ALA	B	4	22.351	50.775	-16.116	0.00	0.00	7
CA	ALA	B	4	23.483	49.923	-16.440	0.00	0.00	6
CB	ALA	B	4	24.439	49.900	-15.247	0.00	0.00	6
C	ALA	B	4	23.094	48.490	-16.774	0.00	0.00	6
O	ALA	B	4	23.937	47.679	-17.164	0.00	0.00	8
N	TYR	B	4	21.823	48.159	-16.611	0.00	0.00	7
CA	TYR	B	4	21.336	46.806	-16.810	0.00	0.00	6
CB	TYR	B	4	20.088	46.602	-15.938	0.00	0.00	6
C	TYR	B	4	20.413	46.522	-14.460	0.00	0.00	6
C	TYR	B	4	20.745	47.655	-13.731	0.00	0.00	6
CE	TYR	B	4	21.048	47.578	-12.383	0.00	0.00	6
C	TYR	B	4	20.391	45.303	-13.795	0.00	0.00	6
CE	TYR	B	4	20.690	45.216	-12.449	0.00	0.00	6
CZ	TYR	B	4	21.014	46.355	-11.747	0.00	0.00	6
O	TYR	B	4	21.313	46.273	-10.407	0.00	0.00	8
C	TYR	B	4	21.059	46.459	-18.261	0.00	0.00	6
O	TYR	B	4	20.554	47.253	-19.049	0.00	0.00	8
N	ALA	B	4	21.370	45.209	-18.607	0.00	0.00	7
CA	ALA	B	4	21.142	44.684	-19.946	0.00	0.00	6
CB	ALA	B	4	22.005	43.456	-20.186	0.00	0.00	6
C	ALA	B	4	19.666	44.352	-20.146	0.00	0.00	6
O	ALA	B	4	19.154	44.407	-21.263	0.00	0.00	8
N	THR	B	4	18.993	43.971	-19.067	0.00	0.00	7
CA	THR	B	4	17.560	43.695	-19.106	0.00	0.00	6
CB	THR	B	4	17.216	42.255	-18.717	0.00	0.00	6
O	THR	B	4	17.923	41.358	-19.587	0.00	0.00	8
C	THR	B	4	15.719	42.013	-18.850	0.00	0.00	6
C	THR	B	4	16.868	44.707	-18.197	0.00	0.00	6
O	THR	B	4	17.208	44.856	-17.024	0.00	0.00	8
N	LYS	B	4	15.919	45.441	-18.768	0.00	0.00	7
CA	LYS	B	4	15.215	46.491	-18.050	0.00	0.00	6
CB	LYS	B	4	15.389	47.815	-18.819	0.00	0.00	6
C	LYS	B	4	16.831	48.251	-19.005	0.00	0.00	6
C	LYS	B	4	17.050	48.954	-20.333	0.00	0.00	6
CE	LYS	B	4	18.371	49.707	-20.339	0.00	0.00	6
NZ	LYS	B	4	19.484	48.873	-20.865	0.00	0.00	7
C	LYS	B	4	13.734	46.220	-17.861	0.00	0.00	6

O	LYS	B	4	13.002	47.106	-17.414	0.00	0.00	8
N	PHE	B	4	13.301	45.009	-18.189	0.00	0.00	7
CA	PHE	B	4	11.887	44.672	-18.067	0.00	0.00	6
CB	PHE	B	4	11.267	44.557	-19.465	0.00	0.00	6
C	PHE	B	4	11.965	43.566	-20.352	0.00	0.00	6
C	PHE	B	4	11.550	42.247	-20.404	0.00	0.00	6
C	PHE	B	4	13.041	43.957	-21.135	0.00	0.00	6
CE	PHE	B	4	12.192	41.332	-21.220	0.00	0.00	6
CE	PHE	B	4	13.689	43.046	-21.946	0.00	0.00	6
CZ	PHE	B	4	13.260	41.735	-21.996	0.00	0.00	6
C	PHE	B	4	11.666	43.382	-17.292	0.00	0.00	6
O	PHE	B	4	12.576	42.577	-17.108	0.00	0.00	8
N	ALA	B	5	10.424	43.181	-16.864	0.00	0.00	7
CA	ALA	B	5	10.032	41.986	-16.135	0.00	0.00	6
CB	ALA	B	5	10.666	41.977	-14.749	0.00	0.00	6
C	ALA	B	5	8.513	41.888	-16.010	0.00	0.00	6
O	ALA	B	5	7.772	42.820	-16.314	0.00	0.00	8
N	GLY	B	5	8.060	40.724	-15.560	0.00	0.00	7
CA	GLY	B	5	6.631	40.512	-15.301	0.00	0.00	6
C	GLY	B	5	6.446	40.886	-13.820	0.00	0.00	6
O	GLY	B	5	6.858	40.138	-12.933	0.00	0.00	8
N	LEU	B	5	5.924	42.082	-13.579	0.00	0.00	7
CA	LEU	B	5	5.763	42.560	-12.212	0.00	0.00	6
CB	LEU	B	5	6.262	44.005	-12.103	0.00	0.00	6
C	LEU	B	5	7.754	44.212	-12.389	0.00	0.00	6
C	LEU	B	5	8.010	45.627	-12.886	0.00	0.00	6
C	LEU	B	5	8.586	43.905	-11.153	0.00	0.00	6
C	LEU	B	5	4.322	42.452	-11.736	0.00	0.00	6
O	LEU	B	5	3.391	42.541	-12.533	0.00	0.00	8
N	VAL	B	5	4.155	42.220	-10.437	0.00	0.00	7
CA	VAL	B	5	2.802	42.166	-9.866	0.00	0.00	6
CB	VAL	B	5	2.748	41.398	-8.547	0.00	0.00	6
C	VAL	B	5	1.428	41.596	-7.817	0.00	0.00	6
C	VAL	B	5	2.966	39.909	-8.810	0.00	0.00	6
C	VAL	B	5	2.356	43.620	-9.731	0.00	0.00	6
O	VAL	B	5	3.072	44.437	-9.153	0.00	0.00	8
N	LYS	B	5	1.232	43.952	-10.349	0.00	0.00	7
CA	LYS	B	5	0.753	45.325	-10.391	0.00	0.00	6
CB	LYS	B	5	0.339	45.647	-11.840	0.00	0.00	6
C	LYS	B	5	1.523	45.696	-12.794	0.00	0.00	6
C	LYS	B	5	1.113	45.408	-14.228	0.00	0.00	6
CE	LYS	B	5	1.623	44.063	-14.705	0.00	0.00	6
NZ	LYS	B	5	3.062	44.089	-15.081	0.00	0.00	7
C	LYS	B	5	-0.391	45.635	-9.444	0.00	0.00	6
O	LYS	B	5	-1.385	44.920	-9.337	0.00	0.00	8
N	ASP	B	5	-0.285	46.789	-8.783	0.00	0.00	7
CA	ASP	B	5	-1.310	47.298	-7.881	0.00	0.00	6
CB	ASP	B	5	-2.588	47.593	-8.678	0.00	0.00	6
C	ASP	B	5	-2.359	48.623	-9.771	0.00	0.00	6
O	ASP	B	5	-1.815	49.702	-9.459	0.00	0.00	8
O	ASP	B	5	-2.682	48.318	-10.940	0.00	0.00	8
C	ASP	B	5	-1.600	46.349	-6.727	0.00	0.00	6
O	ASP	B	5	-2.750	46.016	-6.428	0.00	0.00	8
N	PHE	B	5	-0.549	45.928	-6.037	0.00	0.00	7
CA	PHE	B	5	-0.658	44.970	-4.945	0.00	0.00	6
CB	PHE	B	5	0.677	44.225	-4.825	0.00	0.00	6
C	PHE	B	5	0.791	43.249	-3.696	0.00	0.00	6
C	PHE	B	5	0.037	42.088	-3.672	0.00	0.00	6
C	PHE	B	5	1.674	43.489	-2.653	0.00	0.00	6
CE	PHE	B	5	0.151	41.190	-2.629	0.00	0.00	6
CE	PHE	B	5	1.792	42.594	-1.607	0.00	0.00	6
CZ	PHE	B	5	1.029	41.443	-1.595	0.00	0.00	6
C	PHE	B	5	-1.074	45.599	-3.627	0.00	0.00	6
O	PHE	B	5	-0.444	46.521	-3.115	0.00	0.00	8

Figure 1 - 27

N	ASN	B	5	-2.151	45.071	-3.051	0.00	0.00	7
CA	ASN	B	5	-2.663	45.532	-1.769	0.00	0.00	6
CB	ASN	B	5	-3.948	46.342	-1.930	0.00	0.00	6
C	ASN	B	5	-4.421	46.975	-0.637	0.00	0.00	6
O	ASN	B	5	-5.590	46.855	-0.266	0.00	0.00	8
N	ASN	B	5	-3.525	47.660	0.065	0.00	0.00	7
C	ASN	B	5	-2.914	44.343	-0.842	0.00	0.00	6
O	ASN	B	5	-3.604	43.391	-1.203	0.00	0.00	8
N	CYS	B	5	-2.309	44.399	0.338	0.00	0.00	7
CA	CYS	B	5	-2.467	43.334	1.322	0.00	0.00	6
CB	CYS	B	5	-1.236	42.431	1.347	0.00	0.00	6
SG	CYS	B	5	0.252	43.226	1.997	0.00	0.00	1
C	CYS	B	5	-2.728	43.929	2.699	0.00	0.00	6
O	CYS	B	5	-2.729	43.232	3.709	0.00	0.00	8
N	GLU	B	5	-3.065	45.214	2.722	0.00	0.00	7
CA	GLU	B	5	-3.394	45.936	3.943	0.00	0.00	6
CB	GLU	B	5	-3.775	47.378	3.604	0.00	0.00	6
C	GLU	B	5	-3.621	48.366	4.743	0.00	0.00	6
C	GLU	B	5	-2.414	49.271	4.612	0.00	0.00	6
O	GLU	B	5	-2.406	50.339	5.266	0.00	0.00	8
O	GLU	B	5	-1.469	48.932	3.872	0.00	0.00	8
C	GLU	B	5	-4.520	45.260	4.717	0.00	0.00	6
O	GLU	B	5	-4.445	45.096	5.936	0.00	0.00	8
N	ASP	B	6	-5.547	44.799	4.013	0.00	0.00	7
CA	ASP	B	6	-6.654	44.067	4.601	0.00	0.00	6
CB	ASP	B	6	-7.786	43.855	3.599	0.00	0.00	6
C	ASP	B	6	-7.406	43.958	2.141	0.00	0.00	6
O	ASP	B	6	-7.476	42.929	1.431	0.00	0.00	8
O	ASP	B	6	-7.060	45.066	1.677	0.00	0.00	8
C	ASP	B	6	-6.217	42.726	5.186	0.00	0.00	6
O	ASP	B	6	-6.727	42.320	6.232	0.00	0.00	8
N	ILE	B	6	-5.292	42.034	4.531	0.00	0.00	7
CA	ILE	B	6	-4.814	40.742	4.995	0.00	0.00	6
CB	ILE	B	6	-4.325	39.863	3.824	0.00	0.00	6
C	ILE	B	6	-4.200	38.412	4.270	0.00	0.00	6
C	ILE	B	6	-5.229	39.984	2.600	0.00	0.00	6
C	ILE	B	6	-6.659	39.533	2.774	0.00	0.00	6
C	ILE	B	6	-3.692	40.849	6.020	0.00	0.00	6
O	ILE	B	6	-3.679	40.118	7.013	0.00	0.00	8
N	ILE	B	6	-2.663	41.635	5.720	0.00	0.00	7
CA	ILE	B	6	-1.509	41.805	6.587	0.00	0.00	6
CB	ILE	B	6	-0.185	41.329	5.963	0.00	0.00	6
C	ILE	B	6	0.946	41.398	6.985	0.00	0.00	6
C	ILE	B	6	-0.271	39.907	5.404	0.00	0.00	6
C	ILE	B	6	0.146	39.804	3.952	0.00	0.00	6
C	ILE	B	6	-1.340	43.279	6.962	0.00	0.00	6
O	ILE	B	6	-1.307	44.147	6.089	0.00	0.00	8
N	SER	B	6	-1.176	43.542	8.254	0.00	0.00	7
CA	SER	B	6	-1.027	44.913	8.732	0.00	0.00	6
CB	SER	B	6	-1.109	44.966	1			

N	LYS	B	6	2.286	47.070	10.259	0.00	0.00	7
CA	LYS	B	6	3.206	46.697	11.323	0.00	0.00	6
CB	LYS	B	6	2.497	46.565	12.667	0.00	0.00	6
C	LYS	B	6	1.922	47.844	13.247	0.00	0.00	6
C	LYS	B	6	0.962	47.542	14.390	0.00	0.00	6
CE	LYS	B	6	-0.211	48.508	14.405	0.00	0.00	6
NZ	LYS	B	6	-1.501	47.832	14.094	0.00	0.00	7
C	LYS	B	6	3.836	45.348	10.959	0.00	0.00	6
O	LYS	B	6	5.053	45.206	10.893	0.00	0.00	8
N	GLU	B	6	2.985	44.370	10.663	0.00	0.00	7
CA	GLU	B	6	3.403	43.026	10.303	0.00	0.00	6
CB	GLU	B	6	2.191	42.084	10.348	0.00	0.00	6
C	GLU	B	6	1.842	41.634	11.759	0.00	0.00	6
C	GLU	B	6	2.805	40.594	12.296	0.00	0.00	6
O	GLU	B	6	3.270	40.746	13.444	0.00	0.00	8
O	GLU	B	6	3.100	39.622	11.571	0.00	0.00	8
C	GLU	B	6	4.103	42.913	8.961	0.00	0.00	6
O	GLU	B	6	4.935	42.026	8.749	0.00	0.00	8
N	GLN	B	6	3.833	43.819	8.034	0.00	0.00	7
CA	GLN	B	6	4.432	43.873	6.715	0.00	0.00	6
CB	GLN	B	6	3.810	45.047	5.948	0.00	0.00	6
C	GLN	B	6	3.455	44.788	4.497	0.00	0.00	6
C	GLN	B	6	2.649	45.939	3.918	0.00	0.00	6
O	GLN	B	6	3.186	47.022	3.682	0.00	0.00	8
N	GLN	B	6	1.359	45.711	3.700	0.00	0.00	7
C	GLN	B	6	5.942	44.057	6.731	0.00	0.00	6
O	GLN	B	6	6.651	43.615	5.825	0.00	0.00	8
N	ARG	B	6	6.479	44.703	7.756	0.00	0.00	7
CA	ARG	B	6	7.885	44.986	7.939	0.00	0.00	6
CB	ARG	B	6	8.036	46.018	9.074	0.00	0.00	6
C	ARG	B	6	9.323	46.817	9.005	0.00	0.00	6
C	ARG	B	6	10.089	46.770	10.317	0.00	0.00	6
N	ARG	B	6	11.527	46.897	10.120	0.00	0.00	7
CZ	ARG	B	6	12.168	47.990	9.730	0.00	0.00	6
N	ARG	B	6	11.506	49.112	9.476	0.00	0.00	7
N	ARG	B	6	13.490	47.967	9.589	0.00	0.00	7
C	ARG	B	6	8.747	43.779	8.272	0.00	0.00	6
O	ARG	B	6	9.976	43.834	8.163	0.00	0.00	8
N	LYS	B	6	8.138	42.682	8.698	0.00	0.00	7
CA	LYS	B	6	8.845	41.466	9.047	0.00	0.00	6
CB	LYS	B	6	8.136	40.762	10.211	0.00	0.00	6
C	LYS	B	6	7.765	41.649	11.385	0.00	0.00	6
C	LYS	B	6	7.064	40.835	12.467	0.00	0.00	6
CE	LYS	B	6	6.806	41.674	13.707	0.00	0.00	6
NZ	LYS	B	6	5.642	41.179	14.491	0.00	0.00	7
C	LYS	B	6	8.927	40.481	7.885	0.00	0.00	6
O	LYS	B	6	9.369	39.348	8.094	0.00	0.00	8
N	MET	B	7	8.488	40.866	6.690	0.00	0.00	7
CA	MET	B	7	8.447	39.924	5.584	0.00	0.00	6
CB	MET	B	7	7.059	39.264	5.527	0.00	0.00	6
C	MET	B	7	5.892	40.186	5.822	0.00	0.00	6
SD	MET	B	7	4.290	39.377	5.704	0.00	0.00	1
CE	MET	B	7	4.070	38.756	7.367	0.00	0.00	6
C	MET	B	7	8.777	40.497	4.215	0.00	0.00	6
O	MET	B	7	8.267	41.528	3.787	0.00	0.00	8
N	ASP	B	7	9.641	39.772	3.503	0.00	0.00	7
CA	ASP	B	7	10.018	40.153	2.143	0.00	0.00	6
CB	ASP	B	7	11.102	39.217	1.616	0.00	0.00	6
C	ASP	B	7	11.626	39.596	0.246	0.00	0.00	6
O	ASP	B	7	11.084	39.090	-0.762	0.00	0.00	8
O	ASP	B	7	12.566	40.415	0.170	0.00	0.00	8
C	ASP	B	7	8.766	40.077	1.273	0.00	0.00	6
O	ASP	B	7	7.838	39.332	1.603	0.00	0.00	8
N	ALA	B	7	8.768	40.721	0.115	0.00	0.00	7

C	ALA	B	8	-2.383	33.822	-2.558	0.00	0.00	6
CB	ALA	B	8	-1.272	33.385	-3.500	0.00	0.00	6
C	ALA	B	8	-2.843	32.640	-1.711	0.00	0.00	6
O	ALA	B	8	-3.746	31.904	-2.112	0.00	0.00	8
N	GLY	B	8	-2.218	32.434	-0.555	0.00	0.00	7
CA	GLY	B	8	-2.604	31.380	0.370	0.00	0.00	6
C	GLY	B	8	-3.981	31.650	0.965	0.00	0.00	6
O	GLY	B	8	-4.833	30.763	1.014	0.00	0.00	8
N	VAL	B	8	-4.230	32.898	1.357	0.00	0.00	7
CA	VAL	B	8	-5.528	33.288	1.897	0.00	0.00	6
CB	VAL	B	8	-5.532	34.736	2.405	0.00	0.00	6
C	VAL	B	8	-6.925	35.177	2.836	0.00	0.00	6
C	VAL	B	8	-4.556	34.880	3.570	0.00	0.00	6
C	VAL	B	8	-6.620	33.064	0.859	0.00	0.00	6
O	VAL	B	8	-7.659	32.482	1.179	0.00	0.00	8
N	GLN	B	8	-6.364	33.415	-0.397	0.00	0.00	7
CA	GLN	B	8	-7.290	33.149	-1.485	0.00	0.00	6
CB	GLN	B	8	-6.721	33.632	-2.822	0.00	0.00	6
C	GLN	B	8	-6.689	35.138	-3.007	0.00	0.00	6
C	GLN	B	8	-6.219	35.543	-4.389	0.00	0.00	6
O	GLN	B	8	-6.176	34.726	-5.309	0.00	0.00	8
N	GLN	B	8	-5.860	36.811	-4.554	0.00	0.00	7
C	GLN	B	8	-7.631	31.667	-1.602	0.00	0.00	6
O	GLN	B	8	-8.802	31.315	-1.758	0.00	0.00	8
N	ALA	B	8	-6.629	30.793	-1.539	0.00	0.00	7
CA	ALA	B	8	-6.857	29.358	-1.660	0.00	0.00	6
CB	ALA	B	8	-5.541	28.617	-1.828	0.00	0.00	6
C	ALA	B	8	-7.647	28.802	-0.484	0.00	0.00	6
O	ALA	B	8	-8.519	27.949	-0.673	0.00	0.00	8
N	MET	B	8	-7.360	29.274	0.724	0.00	0.00	7
CA	MET	B	8	-8.113	28.856	1.902	0.00	0.00	6
CB	MET	B	8	-7.490	29.432	3.172	0.00	0.00	6
C	MET	B	8	-6.228	28.709	3.621	0.00	0.00	6
SD	MET	B	8	-6.445	26.925	3.753	0.00	0.00	1
CE	MET	B	8	-6.387	26.701	5.528	0.00	0.00	6
C	MET	B	8	-9.574	29.266	1.757	0.00	0.00	6
O	MET	B	8	-10.478	28.445	1.919	0.00	0.00	8
N	GLN	B	8	-9.809	30.522	1.397	0.00	0.00	7
CA	GLN	B	8	-11.155	31.043	1.192	0.00	0.00	6
CB	GLN	B	8	-11.101	32.552	0.925	0.00	0.00	6
C	GLN	B	8	-10.844	33.369	2.182	0.00	0.00	6
C	GLN	B	8	-10.738	34.853	1.924	0.00	0.00	6
O	GLN	B	8	-10.769	35.311	0.781	0.00	0.00	8
N	GLN	B	8	-10.614	35.637	2.991	0.00	0.00	7
C	GLN	B	8	-11.886	30.313	0.077	0.00	0.00	6
O	GLN	B	8	-12.990	29.807	0.293	0.00	0.00	8
N	ASP	B	8	-11.248	30.116	-1.071	0.00	0.00	7
CA	ASP	B	8	-11.840	29.371	-2.171	0.00	0.00	6
CB	ASP	B	8	-10.878	29.284	-3.364	0.00	0.00	6
C	ASP	B	8	-11.590	28.837	-4.627	0.00	0.00	6
O	ASP	B	8	-12.739	29.283	-4.836	0.00	0.00	8
O	ASP	B	8	-11.029	28.050	-5.413	0.00	0.00	8
C	ASP	B	8	-12.257	27.955	-1.785	0.00	0.00	6
O	ASP	B	8	-13.279	27.457	-2.261	0.00	0.00	8
N	SER	B	8	-11.451	27.269	-0.987	0.00	0.00	7
CA	SER	B	8	-11.687	25.893	-0.605	0.00	0.00	6
CB	SER	B	8	-10.467	25.349	0.151	0.00	0.00	6
O	SER	B	8	-10.360	25.936	1.435	0.00	0.00	8
C	SER	B	8	-12.934	25.657	0.235	0.00	0.00	6
O	SER	B	8	-13.620	24.651	0.031	0.00	0.00	8
N	GLY	B	8	-13.196	26.528	1.203	0.00	0.00	7
CA	GLY	B	8	-14.320	26.296	2.114	0.00	0.00	6
C	GLY	B	8	-13.881	25.231	3.124	0.00	0.00	6
O	GLY	B	8	-14.413	24.126	3.181	0.00	0.00	8

Figure 1 - 29

N	LEU	B	9	-12.800	25.551	3.826	0.00	0.00	7
CA	LEU	B	9	-12.265	24.680	4.861	0.00	0.00	6
CB	LEU	B	9	-10.779	24.409	4.677	0.00	0.00	6
C	LEU	B	9	-10.302	22.986	4.394	0.00	0.00	6
C	LEU	B	9	-10.926	21.966	5.334	0.00	0.00	6
C	LEU	B	9	-10.574	22.608	2.943	0.00	0.00	6
C	LEU	B	9	-12.507	25.349	6.216	0.00	0.00	6
O	LEU	B	9	-12.209	26.531	6.384	0.00	0.00	8
N	GLU	B	9	-13.164	24.627	7.112	0.00	0.00	7
CA	GLU	B	9	-13.346	25.130	8.474	0.00	0.00	6
CB	GLU	B	9	-14.753	24.868	8.989	0.00	0.00	6
C	GLU	B	9	-15.849	25.580	8.213	0.00	0.00	6
C	GLU	B	9	-16.839	26.303	9.104	0.00	0.00	6
O	GLU	B	9	-17.285	25.715	10.113	0.00	0.00	8
O	GLU	B	9	-17.179	27.465	8.797	0.00	0.00	8
C	GLU	B	9	-12.279	24.461	9.339	0.00	0.00	6
O	GLU	B	9	-12.201	23.231	9.355	0.00	0.00	8
N	ILE	B	9	-11.401	25.263	9.933	0.00	0.00	7
CA	ILE	B	9	-10.330	24.696	10.753	0.00	0.00	6
CB	ILE	B	9	-9.003	25.449	10.595	0.00	0.00	6
C	ILE	B	9	-7.980	25.028	11.642	0.00	0.00	6
C	ILE	B	9	-8.425	25.204	9.195	0.00	0.00	6
C	ILE	B	9	-8.612	26.358	8.239	0.00	0.00	6
C	ILE	B	9	-10.771	24.645	12.212	0.00	0.00	6
O	ILE	B	9	-10.993	25.660	12.864	0.00	0.00	8
N	THR	B	9	-10.950	23.422	12.698	0.00	0.00	7
CA	THR	B	9	-11.365	23.176	14.070	0.00	0.00	6
CB	THR	B	9	-12.591	22.241	14.128	0.00	0.00	6
O	THR	B	9	-12.229	20.972	13.563	0.00	0.00	8
C	THR	B	9	-13.772	22.810	13.365	0.00	0.00	6
C	THR	B	9	-10.245	22.505	14.854	0.00	0.00	6
O	THR	B	9	-9.318	21.938	14.274	0.00	0.00	8
N	GLU	B	9	-10.342	22.519	16.180	0.00	0.00	7
CA	GLU	B	9	-9.350	21.894	17.050	0.00	0.00	6
CB	GLU	B	9	-9.745	22.075	18.517	0.00	0.00	6
C	GLU	B	9	-8.854	21.362	19.515	0.00	0.00	6
C	GLU	B	9	-8.091	22.295	20.431	0.00	0.00	6
O	GLU	B	9	-6.877	22.071	20.630	0.00	0.00	8
O	GLU	B	9	-8.696	23.252	20.959	0.00	0.00	8
C	GLU	B	9	-9.159	20.418	16.722	0.00	0.00	6
O	GLU	B	9	-8.050	19.886	16.829	0.00	0.00	8
N	GLU	B	9	-10.204	19.729	16.283	0.00	0.00	7
CA	GLU	B	9	-10.171	18.345	15.864	0.00	0.00	6
CB	GLU	B	9	-11.575	17.732	15.975	0.00	0.00	6
C	GLU	B	9	-11.800	16.947	17.254	0.00	0.00	6
C	GLU	B	9	-13.188	17.128	17.834	0.00	0.00	6
O	GLU	B	9	-14.097	16.358	17.458	0.00	0.00	8
O	GLU	B	9	-13.370	18.034	18.674	0.00	0.00	8
C	GLU	B	9	-9.670	18.170	14.432	0.00	0.00	6
O	GLU	B	9	-9.491	17.043	13.964	0.00	0.00	8
N	ASN	B	9	-9.451	19.258	13.708	0.00	0.00	7
CA	ASN	B	9	-8.967	19.250	12.345	0.00	0.00	6
CB	ASN	B	9	-9.751	20.278	11.509	0.00	0.00	6
C	ASN	B	9	-10.403	19.694	10.279	0.00	0.00	6
O	ASN	B	9	-10.214	18.522	9.952	0.00	0.00	8
N	ASN	B	9	-11.188	20.509	9.584	0.00	0.00	7
C	ASN	B	9	-7.497	19.629	12.209	0.00	0.00	6
O	ASN	B	9	-6.767	19.093	11.376	0.00	0.00	8
N	ALA	B	9	-7.065	20.621	12.974	0.00	0.00	7
CA	ALA	B	9	-5.737	21.205	12.898	0.00	0.00	6
CB	ALA	B	9	-5.410	21.900	14.219	0.00	0.00	6
C	ALA	B	9	-4.627	20.235	12.535	0.00	0.00	6
O	ALA	B	9	-3.912	20.381	11.545	0.00	0.00	8
N	THR	B	9	-4.462	19.187	13.317	0.00	0.00	7

CA	THR	B	9	-3.494	18.120	13.183	0.00	0.00	6
CB	THR	B	9	-3.849	17.091	14.293	0.00	0.00	6
O	THR	B	9	-3.158	17.483	15.494	0.00	0.00	8
C	THR	B	9	-3.510	15.649	13.985	0.00	0.00	6
C	THR	B	9	-3.392	17.455	11.826	0.00	0.00	6
O	THR	B	9	-2.336	16.879	11.520	0.00	0.00	8
N	ARG	B	9	-4.417	17.469	10.983	0.00	0.00	7
CA	ARG	B	9	-4.390	16.835	9.680	0.00	0.00	6
CB	ARG	B	9	-5.674	16.018	9.462	0.00	0.00	6
C	ARG	B	9	-5.976	14.996	10.544	0.00	0.00	6
C	ARG	B	9	-4.989	13.839	10.499	0.00	0.00	6
N	ARG	B	9	-5.164	13.029	9.300	0.00	0.00	7
CZ	ARG	B	9	-4.248	12.221	8.785	0.00	0.00	6
N	ARG	B	9	-3.058	12.093	9.357	0.00	0.00	7
N	ARG	B	9	-4.525	11.530	7.686	0.00	0.00	7
C	ARG	B	9	-4.224	17.795	8.512	0.00	0.00	6
O	ARG	B	9	-4.283	17.365	7.356	0.00	0.00	8
N	ILE	B	1	-4.106	19.091	8.777	0.00	0.00	7
CA	ILE	B	1	-3.917	20.072	7.716	0.00	0.00	6
CB	ILE	B	1	-4.981	21.183	7.700	0.00	0.00	6
C	ILE	B	1	-4.898	21.961	6.389	0.00	0.00	6
C	ILE	B	1	-6.399	20.638	7.890	0.00	0.00	6
C	ILE	B	1	-7.341	21.612	8.564	0.00	0.00	6
C	ILE	B	1	-2.543	20.728	7.839	0.00	0.00	6
O	ILE	B	1	-2.204	21.247	8.904	0.00	0.00	8
N	GLY	B	1	-1.772	20.711	6.756	0.00	0.00	7
CA	GLY	B	1	-0.455	21.336	6.771	0.00	0.00	6
C	GLY	B	1	-0.164	22.114	5.493	0.00	0.00	6
O	GLY	B	1	-1.084	22.519	4.781	0.00	0.00	8
N	ALA	B	1	1.123	22.287	5.193	0.00	0.00	7
CA	ALA	B	1	1.544	23.043	4.025	0.00	0.00	6
CB	ALA	B	1	1.703	24.508	4.437	0.00	0.00	6
C	ALA	B	1	2.845	22.569	3.390	0.00	0.00	6
O	ALA	B	1	3.731	21.988	4.008	0.00	0.00	8
N	ALA	B	1	2.964	22.834	2.093	0.00	0.00	7
CA	ALA	B	1	4.129	22.478	1.294	0.00	0.00	6
CB	ALA	B	1	3.955	21.139	0.604	0.00	0.00	6
C	ALA	B	1	4.359	23.608	0.290	0.00	0.00	6
O	ALA	B	1	3.925	23.556	-0.858	0.00	0.00	8
N	ILE	B	1	4.901	24.712	0.799	0.00	0.00	7
CA	ILE	B	1	5.111	25.917	0.008	0.00	0.00	6
CB	ILE	B	1	4.382	27.134	0.609	0.00	0.00	6
C	ILE	B	1	4.641	28.386	-0.218	0.00	0.00	6
C	ILE	B	1	2.875	26.885	0.727	0.00	0.00	6
C	ILE	B	1	2.201	27.727	1.789	0.00	0.00	6
C	ILE	B	1	6.599	26.245	-0.103	0.00	0.00	6
O	ILE	B	1	7.283	26.357	0.912	0.00	0.00	8
N	GLY	B	1	7.071	26.480	-1.321	0.00	0.00	7
CA	GLY	B	1	8.464	26.805	-1.546	0.00	0.00	6
C	GLY	B	1	8.689	28.092	-2.326	0.00	0.00	6
O	GLY	B	1	7.803	28.887	-2.619	0.00	0.00	8
N	SER	B	1	9.955	28.293	-2.663	0.00	0.00	7
CA	SER	B	1	10.463	29.437	-3.400	0.00	0.00	6
CB	SER	B	1	10.521	30.675	-2.511	0.00	0.00	6
O	SER	B	1	10.955	31.817	-3.224	0.00	0.00	8
C	SER	B	1	11.864	29.074	-3.895	0.00	0.00	6
O	SER	B	1	12.571	28.343	-3.198	0.00	0.00	8
N	GLY	B	1	12.255	29.560	-5.062	0.00	0.00	7
CA	GLY	B	1	13.558	29.254	-5.619	0.00	0.00	6
C	GLY	B	1	14.702	30.060	-5.036	0.00	0.00	6
O	GLY	B	1	15.795	29.516	-4.846	0.00	0.00	8
N	ILE	B	1	14.500	31.353	-4.800	0.00	0.00	7
CA	ILE	B	1	15.555	32.223	-4.284	0.00	0.00	6
CB	ILE	B	1	15.897	33.314	-5.317	0.00	0.00	6

Figure 1 - 30

C	ILE	B	1	16.794	34.404	-4.750	0.00	0.00	6
C	ILE	B	1	16.591	32.700	-6.544	0.00	0.00	6
C	ILE	B	1	16.491	33.542	-7.796	0.00	0.00	6
C	ILE	B	1	15.199	32.836	-2.938	0.00	0.00	6
O	ILE	B	1	16.082	33.200	-2.153	0.00	0.00	8
N	GLY	B	1	13.913	32.958	-2.623	0.00	0.00	7
CA	GLY	B	1	13.500	33.524	-1.345	0.00	0.00	6
C	GLY	B	1	13.749	35.023	-1.274	0.00	0.00	6
O	GLY	B	1	13.728	35.733	-2.279	0.00	0.00	8
N	GLY	B	1	13.868	35.559	-0.062	0.00	0.00	7
CA	GLY	B	1	13.870	36.971	0.218	0.00	0.00	6
C	GLY	B	1	15.050	37.802	-0.223	0.00	0.00	6
O	GLY	B	1	15.661	38.511	0.585	0.00	0.00	8
N	LEU	B	1	15.285	37.900	-1.526	0.00	0.00	7
CA	LEU	B	1	16.398	38.625	-2.104	0.00	0.00	6
CB	LEU	B	1	16.437	38.408	-3.622	0.00	0.00	6
C	LEU	B	1	17.663	37.729	-4.225	0.00	0.00	6
C	LEU	B	1	17.647	37.859	-5.744	0.00	0.00	6
C	LEU	B	1	18.962	38.287	-3.670	0.00	0.00	6
C	LEU	B	1	16.332	40.119	-1.822	0.00	0.00	6
O	LEU	B	1	17.336	40.749	-1.493	0.00	0.00	8
N	GLY	B	1	15.138	40.687	-1.966	0.00	0.00	7
CA	GLY	B	1	14.920	42.106	-1.717	0.00	0.00	6
C	GLY	B	1	15.413	42.510	-0.333	0.00	0.00	6
O	GLY	B	1	16.245	43.408	-0.215	0.00	0.00	8
N	LEU	B	1	15.004	41.772	0.696	0.00	0.00	7
CA	LEU	B	1	15.384	42.075	2.069	0.00	0.00	6
CB	LEU	B	1	14.380	41.456	3.045	0.00	0.00	6
C	LEU	B	1	13.469	42.434	3.794	0.00	0.00	6
C	LEU	B	1	12.982	43.576	2.917	0.00	0.00	6
C	LEU	B	1	12.272	41.709	4.396	0.00	0.00	6
C	LEU	B	1	16.822	41.718	2.403	0.00	0.00	6
O	LEU	B	1	17.408	42.358	3.288	0.00	0.00	8
N	ILE	B	1	17.433	40.762	1.707	0.00	0.00	7
CA	ILE	B	1	18.834	40.428	1.959	0.00	0.00	6
CB	ILE	B	1	19.264	39.105	1.314	0.00	0.00	6
C	ILE	B	1	20.776	38.921	1.351	0.00	0.00	6
C	ILE	B	1	18.579	37.928	2.019	0.00	0.00	6
C	ILE	B	1	18.555	36.654	1.206	0.00	0.00	6
C	ILE	B	1	19.716	41.575	1.461	0.00	0.00	6
O	ILE	B	1	20.702	41.937	2.103	0.00	0.00	8
N	GLU	B	1	19.338	42.165	0.332	0.00	0.00	7
CA	GLU	B	1	20.048	43.316	-0.209	0.00	0.00	6
CB	GLU	B	1	19.511	43.682	-1.590	0.00	0.00	6
C	GLU	B	1	19.818	42.650	-2.666	0.00	0.00	6
C	GLU	B	1	19.261	43.083	-4.010	0.00	0.00	6
O	GLU	B	1	18.715	42.231	-4.736	0.00	0.00	8
O	GLU	B	1	19.370	44.288	-4.318	0.00	0.00	8
C	GLU	B	1	19.955	44.515	0.727	0		

N	ASN	B	1	17.280	42.501	5.940	0.00	0.00	7
C	ASN	B	1	21.570	44.367	4.958	0.00	0.00	6
O	ASN	B	1	22.333	44.848	5.801	0.00	0.00	8
N	HIS	B	1	22.005	43.840	3.811	0.00	0.00	7
CA	HIS	B	1	23.431	43.856	3.503	0.00	0.00	6
CB	HIS	B	1	23.819	43.004	2.295	0.00	0.00	6
C	HIS	B	1	25.315	42.861	2.216	0.00	0.00	6
C	HIS	B	1	26.222	43.348	1.343	0.00	0.00	6
N	HIS	B	1	26.030	42.144	3.151	0.00	0.00	7
CE	HIS	B	1	27.316	42.190	2.852	0.00	0.00	6
N	HIS	B	1	27.457	42.915	1.755	0.00	0.00	7
C	HIS	B	1	23.889	45.303	3.321	0.00	0.00	6
O	HIS	B	1	24.898	45.713	3.898	0.00	0.00	8
N	THR	B	1	23.091	46.103	2.620	0.00	0.00	7
CA	THR	B	1	23.383	47.523	2.448	0.00	0.00	6
CB	THR	B	1	22.322	48.196	1.562	0.00	0.00	6
O	THR	B	1	22.311	47.533	0.288	0.00	0.00	8
C	THR	B	1	22.621	49.671	1.345	0.00	0.00	6
C	THR	B	1	23.500	48.228	3.792	0.00	0.00	6
O	THR	B	1	24.478	48.942	4.033	0.00	0.00	8
N	SER	B	1	22.553	47.994	4.695	0.00	0.00	7
CA	SER	B	1	22.625	48.540	6.047	0.00	0.00	6
CB	SER	B	1	21.426	48.068	6.870	0.00	0.00	6
O	SER	B	1	20.215	48.456	6.236	0.00	0.00	8
C	SER	B	1	23.939	48.154	6.711	0.00	0.00	6
O	SER	B	1	24.722	49.019	7.100	0.00	0.00	8
N	LEU	B	1	24.244	46.863	6.777	0.00	0.00	7
CA	LEU	B	1	25.484	46.363	7.350	0.00	0.00	6
CB	LEU	B	1	25.569	44.846	7.172	0.00	0.00	6
C	LEU	B	1	26.914	44.158	7.405	0.00	0.00	6
C	LEU	B	1	27.242	44.061	8.887	0.00	0.00	6
C	LEU	B	1	26.922	42.773	6.770	0.00	0.00	6
C	LEU	B	1	26.720	47.037	6.775	0.00	0.00	6
O	LEU	B	1	27.612	47.426	7.535	0.00	0.00	8
N	MET	B	1	26.808	47.199	5.461	0.00	0.00	7
CA	MET	B	1	27.955	47.832	4.826	0.00	0.00	6
CB	MET	B	1	27.840	47.751	3.301	0.00	0.00	6
C	MET	B	1	28.732	46.686	2.680	0.00	0.00	6
SD	MET	B	1	28.571	46.613	0.886	0.00	0.00	1
CE	MET	B	1	29.873	47.738	0.383	0.00	0.00	6
C	MET	B	1	28.141	49.285	5.246	0.00	0.00	6
O	MET	B	1	29.272	49.742	5.426	0.00	0.00	8
N	ASN	B	1	27.047	50.023	5.396	0.00	0.00	7
CA	ASN	B	1	27.099	51.420	5.779	0.00	0.00	6
CB	ASN	B	1	25.961	52.184	5.088	0.00	0.00	6
C	ASN	B	1	26.056	52.193	3.581	0.00	0.00	6
O	ASN	B	1	25.032	52.318	2.904	0.00	0.00	8
N	ASN	B	1	27.260	52.066	3.037	0.00	0.00	7
C	ASN	B	1	26.985	51.668	7.277	0.00	0.00	6

Figure 1 - 31

C	ALA	B	1	14.257	24.163	-4.180	0.00	0.00	6
O	ALA	B	1	15.430	23.831	-4.015	0.00	0.00	8
N	THR	B	1	13.619	24.005	-5.336	0.00	0.00	7
CA	THR	B	1	14.295	23.435	-6.499	0.00	0.00	6
CB	THR	B	1	13.706	22.064	-6.879	0.00	0.00	6
O	THR	B	1	12.282	22.111	-6.725	0.00	0.00	8
C	THR	B	1	14.265	20.963	-5.992	0.00	0.00	6
C	THR	B	1	14.225	24.390	-7.684	0.00	0.00	6
O	THR	B	1	13.789	24.006	-8.770	0.00	0.00	8
N	ALA	B	1	14.611	25.645	-7.453	0.00	0.00	7
CA	ALA	B	1	14.614	26.639	-8.530	0.00	0.00	6
CB	ALA	B	1	15.804	26.381	-9.445	0.00	0.00	6
C	ALA	B	1	13.303	26.601	-9.297	0.00	0.00	6
O	ALA	B	1	12.228	26.596	-8.690	0.00	0.00	8
N	CYS	B	1	13.347	26.441	-10.615	0.00	0.00	7
CA	CYS	B	1	12.193	26.376	-11.482	0.00	0.00	6
CB	CYS	B	1	12.628	26.275	-12.957	0.00	0.00	6
SG	CYS	B	1	14.176	27.109	-13.348	0.00	0.00	1
C	CYS	B	1	11.226	25.225	-11.252	0.00	0.00	6
O	CYS	B	1	10.137	25.253	-11.841	0.00	0.00	8
N	THR	B	1	11.590	24.199	-10.504	0.00	0.00	7
CA	THR	B	1	10.719	23.048	-10.288	0.00	0.00	6
CB	THR	B	1	11.539	21.749	-10.439	0.00	0.00	6
O	THR	B	1	12.396	21.886	-11.585	0.00	0.00	8
C	THR	B	1	10.650	20.535	-10.627	0.00	0.00	6
C	THR	B	1	10.032	23.098	-8.938	0.00	0.00	6
O	THR	B	1	9.161	22.283	-8.628	0.00	0.00	8
N	SER	B	1	10.337	24.113	-8.140	0.00	0.00	7
CA	SER	B	1	9.812	24.266	-6.795	0.00	0.00	6
CB	SER	B	1	10.152	25.653	-6.239	0.00	0.00	6
O	SER	B	1	11.536	25.806	-6.014	0.00	0.00	8
C	SER	B	1	8.307	24.060	-6.707	0.00	0.00	6
O	SER	B	1	7.817	23.238	-5.928	0.00	0.00	8
N	GLY	B	1	7.553	24.825	-7.490	0.00	0.00	7
CA	GLY	B	1	6.101	24.743	-7.493	0.00	0.00	6
C	GLY	B	1	5.595	23.335	-7.766	0.00	0.00	6
O	GLY	B	1	4.639	22.887	-7.132	0.00	0.00	8
N	VAL	B	1	6.179	22.652	-8.744	0.00	0.00	7
CA	VAL	B	1	5.760	21.301	-9.104	0.00	0.00	6
CB	VAL	B	1	6.323	20.917	-10.485	0.00	0.00	6
C	VAL	B	1	6.367	19.415	-10.713	0.00	0.00	6
C	VAL	B	1	5.496	21.585	-11.579	0.00	0.00	6
C	VAL	B	1	6.160	20.281	-8.048	0.00	0.00	6
O	VAL	B	1	5.406	19.338	-7.792	0.00	0.00	8
N	HIS	B	1	7.331	20.442	-7.442	0.00	0.00	7
CA	HIS	B	1	7.801	19.513	-6.424	0.00	0.00	6
CB	HIS	B	1	9.283	19.738	-6.120	0.00	0.00	6
C	HIS	B	1	10.227	19.073	-7.069	0.00	0.00	6
C	HIS	B	1	10.065	18.056	-7.947	0.00	0.00	6
N	HIS	B	1	11.548	19.464	-7.180	0.00	0.00	7
CE	HIS	B	1	12.149	18.717	-8.085	0.00	0.00	6
N	HIS	B	1	11.273	17.856	-8.571	0.00	0.00	7
C	HIS	B	1	6.988	19.628	-5.138	0.00	0.00	6
O	HIS	B	1	6.696	18.622	-4.489	0.00	0.00	8
N	ASN	B	1	6.653	20.858	-4.760	0.00	0.00	7
CA	ASN	B	1	5.874	21.100	-3.551	0.00	0.00	6
CB	ASN	B	1	5.824	22.595	-3.249	0.00	0.00	6
C	ASN	B	1	7.045	23.130	-2.535	0.00	0.00	6
O	ASN	B	1	7.850	23.876	-3.102	0.00	0.00	8
N	ASN	B	1	7.210	22.772	-1.268	0.00	0.00	7
C	ASN	B	1	4.472	20.516	-3.684	0.00	0.00	6
O	ASN	B	1	4.023	19.748	-2.832	0.00	0.00	8
N	ILE	B	1	3.796	20.808	-4.791	0.00	0.00	7
CA	ILE	B	1	2.461	20.283	-5.057	0.00	0.00	6

CB	ILE	B	1	1.889	20.822	-6.382	0.00	0.00	6
C	ILE	B	1	0.616	20.091	-6.787	0.00	0.00	6
C	ILE	B	1	1.623	22.325	-6.258	0.00	0.00	6
C	ILE	B	1	1.353	23.023	-7.570	0.00	0.00	6
C	ILE	B	1	2.446	18.758	-5.061	0.00	0.00	6
O	ILE	B	1	1.580	18.154	-4.427	0.00	0.00	8
N	GLY	B	1	3.384	18.133	-5.762	0.00	0.00	7
CA	GLY	B	1	3.472	16.684	-5.812	0.00	0.00	6
C	GLY	B	1	3.809	16.032	-4.479	0.00	0.00	6
O	GLY	B	1	3.271	14.959	-4.179	0.00	0.00	8
N	HIS	B	1	4.669	16.644	-3.659	0.00	0.00	7
CA	HIS	B	1	5.026	16.030	-2.374	0.00	0.00	6
CB	HIS	B	1	6.437	16.407	-1.924	0.00	0.00	6
C	HIS	B	1	7.414	15.486	-2.612	0.00	0.00	6
C	HIS	B	1	7.712	14.188	-2.381	0.00	0.00	6
N	HIS	B	1	8.157	15.865	-3.705	0.00	0.00	7
CE	HIS	B	1	8.893	14.846	-4.108	0.00	0.00	6
N	HIS	B	1	8.641	13.816	-3.321	0.00	0.00	7
C	HIS	B	1	3.927	16.250	-1.352	0.00	0.00	6
O	HIS	B	1	3.717	15.434	-0.451	0.00	0.00	8
N	ALA	B	1	3.120	17.291	-1.551	0.00	0.00	7
CA	ALA	B	1	1.950	17.523	-0.711	0.00	0.00	6
CB	ALA	B	1	1.309	18.858	-1.039	0.00	0.00	6
C	ALA	B	1	0.957	16.381	-0.957	0.00	0.00	6
O	ALA	B	1	0.366	15.835	-0.027	0.00	0.00	8
N	ALA	B	1	0.830	15.965	-2.216	0.00	0.00	7
CA	ALA	B	1	-0.014	14.846	-2.605	0.00	0.00	6
CB	ALA	B	1	-0.214	14.809	-4.111	0.00	0.00	6
C	ALA	B	1	0.554	13.522	-2.103	0.00	0.00	6
O	ALA	B	1	-0.207	12.678	-1.626	0.00	0.00	8
N	ARG	B	1	1.874	13.351	-2.173	0.00	0.00	7
CA	ARG	B	1	2.492	12.133	-1.648	0.00	0.00	6
CB	ARG	B	1	3.989	12.067	-1.913	0.00	0.00	6
C	ARG	B	1	4.401	11.956	-3.365	0.00	0.00	6
C	ARG	B	1	4.151	10.572	-3.938	0.00	0.00	6
N	ARG	B	1	4.957	10.308	-5.126	0.00	0.00	7
CZ	ARG	B	1	4.522	10.309	-6.379	0.00	0.00	6
N	ARG	B	1	3.249	10.571	-6.653	0.00	0.00	7
N	ARG	B	1	5.356	10.051	-7.383	0.00	0.00	7
C	ARG	B	1	2.214	12.059	-0.146	0.00	0.00	6
O	ARG	B	1	1.649	11.071	0.322	0.00	0.00	8
N	ILE	B	1	2.447	13.162	0.571	0.00	0.00	7
CA	ILE	B	1	2.099	13.235	1.987	0.00	0.00	6
CB	ILE	B	1	2.372	14.616	2.602	0.00	0.00	6
C	ILE	B	1	1.809	14.724	4.014	0.00	0.00	6
C	ILE	B	1	3.875	14.919	2.636	0.00	0.00	6
C	ILE	B	1	4.196	16.360	2.989	0.00	0.00	6
C	ILE	B	1	0.643	12.838	2.206	0.00	0.00	6
O	ILE	B	1	0.373	11.945	3.013	0.00	0.00	8
N	ILE	B	1	-0.292	13.468	1.498	0.00	0.00	7
CA	ILE	B	1	-1.708	13.143	1.645	0.00	0.00	6
CB	ILE	B	1	-2.595	14.047	0.770	0.00	0.00	6
C	ILE	B	1	-4.000	13.490	0.605	0.00	0.00	6
C	ILE	B	1	-2.638	15.440	1.408	0.00	0.00	6
C	ILE	B	1	-3.382	16.479	0.614	0.00	0.00	6
C	ILE	B	1	-1.995	11.678	1.362	0.00	0.00	6
O	ILE	B	1	-2.629	11.012	2.183	0.00	0.00	8
N	ALA	B	1	-1.469	11.137	0.271	0.00	0.00	7
CA	ALA	B	1	-1.659	9.743	-0.091	0.00	0.00	6
CB	ALA	B	1	-1.078	9.497	-1.479	0.00	0.00	6
C	ALA	B	1	-1.059	8.761	0.908	0.00	0.00	6
O	ALA	B	1	-1.522	7.620	1.009	0.00	0.00	8
N	TYR	B	1	-0.031	9.162	1.642	0.00	0.00	7
CA	TYR	B	1	0.606	8.329	2.645	0.00	0.00	6

Figure 1 - 34

C	GLY	B	1	18.231	39.294	-10.841	0.00	0.00	6
O	GLY	B	1	18.482	38.368	-11.616	0.00	0.00	8
N	VAL	B	1	18.012	40.540	-11.257	0.00	0.00	7
CA	VAL	B	1	18.114	40.877	-12.680	0.00	0.00	6
CB	VAL	B	1	17.522	42.254	-13.000	0.00	0.00	6
C	VAL	B	1	17.585	42.548	-14.492	0.00	0.00	6
C	VAL	B	1	16.080	42.340	-12.516	0.00	0.00	6
C	VAL	B	1	19.580	40.788	-13.100	0.00	0.00	6
O	VAL	B	1	19.934	40.087	-14.046	0.00	0.00	8
N	GLY	B	2	20.452	41.426	-12.326	0.00	0.00	7
CA	GLY	B	2	21.880	41.395	-12.580	0.00	0.00	6
C	GLY	B	2	22.468	39.993	-12.607	0.00	0.00	6
O	GLY	B	2	23.247	39.675	-13.505	0.00	0.00	8
N	GLY	B	2	22.151	39.157	-11.627	0.00	0.00	7
CA	GLY	B	2	22.680	37.817	-11.495	0.00	0.00	6
C	GLY	B	2	22.380	36.909	-12.672	0.00	0.00	6
O	GLY	B	2	23.254	36.212	-13.187	0.00	0.00	8
N	PHE	B	2	21.128	36.914	-13.116	0.00	0.00	7
CA	PHE	B	2	20.705	36.129	-14.269	0.00	0.00	6
CB	PHE	B	2	19.188	35.986	-14.314	0.00	0.00	6
C	PHE	B	2	18.629	34.898	-13.445	0.00	0.00	6
C	PHE	B	2	17.786	35.206	-12.390	0.00	0.00	6
C	PHE	B	2	18.935	33.568	-13.683	0.00	0.00	6
CE	PHE	B	2	17.263	34.211	-11.585	0.00	0.00	6
CE	PHE	B	2	18.415	32.567	-12.885	0.00	0.00	6
CZ	PHE	B	2	17.576	32.892	-11.835	0.00	0.00	6
C	PHE	B	2	21.222	36.822	-15.531	0.00	0.00	6
O	PHE	B	2	21.633	36.184	-16.493	0.00	0.00	8
N	GLY	B	2	21.309	38.148	-15.481	0.00	0.00	7
CA	GLY	B	2	21.920	38.965	-16.513	0.00	0.00	6
C	GLY	B	2	23.391	38.623	-16.716	0.00	0.00	6
O	GLY	B	2	23.875	38.526	-17.845	0.00	0.00	8
N	ALA	B	2	24.114	38.396	-15.625	0.00	0.00	7
CA	ALA	B	2	25.522	38.052	-15.617	0.00	0.00	6
CB	ALA	B	2	26.053	38.085	-14.186	0.00	0.00	6
C	ALA	B	2	25.826	36.697	-16.238	0.00	0.00	6
O	ALA	B	2	26.920	36.477	-16.760	0.00	0.00	8
N	ALA	B	2	24.863	35.783	-16.211	0.00	0.00	7
CA	ALA	B	2	24.986	34.472	-16.825	0.00	0.00	6
CB	ALA	B	2	24.191	33.446	-16.026	0.00	0.00	6
C	ALA	B	2	24.497	34.494	-18.270	0.00	0.00	6
O	ALA	B	2	24.478	33.476	-18.963	0.00	0.00	8
N	ARG	B	2	24.004	35.644	-18.722	0.00	0.00	7
CA	ARG	B	2	23.499	35.835	-20.070	0.00	0.00	6
CB	ARG	B	2	24.620	35.601	-21.090	0.00	0.00	6
C	ARG	B	2	25.718	36.653	-21.079	0.00	0.00	6
C	ARG	B	2	26.575	36.597	-22.337	0.00	0.00	6
N	ARG	B	2	25.762	36.371	-23.526	0.00	0.00	7
CZ	ARG	B	2	25.831	35.321	-24.333	0.00	0.00	6
N	ARG	B	2	25.011	35.258	-25.377	0.00	0.00	7
N	ARG	B	2	26.699	34.341	-24.113	0.00	0.00	7
C	ARG	B	2	22.308	34.934	-20.376	0.00	0.00	6
O	ARG	B	2	22.108	34.513	-21.515	0.00	0.00	8
N	ALA	B	2	21.458	34.698	-19.386	0.00	0.00	7
CA	ALA	B	2	20.327	33.792	-19.508	0.00	0.00	6
CB	ALA	B	2	20.175	33.000	-18.211	0.00	0.00	6
C	ALA	B	2	19.029	34.535	-19.798	0.00	0.00	6
O	ALA	B	2	18.018	33.936	-20.149	0.00	0.00	8
N	LEU	B	2	19.068	35.847	-19.625	0.00	0.00	7
CA	LEU	B	2	17.911	36.706	-19.813	0.00	0.00	6
CB	LEU	B	2	17.986	37.834	-18.780	0.00	0.00	6
C	LEU	B	2	17.015	37.916	-17.612	0.00	0.00	6
C	LEU	B	2	16.630	36.561	-17.050	0.00	0.00	6
C	LEU	B	2	17.615	38.786	-16.505	0.00	0.00	6

C	LEU	B	2	17.844	37.339	-21.197	0.00	0.00	6
O	LEU	B	2	18.868	37.677	-21.784	0.00	0.00	8
N	SER	B	2	16.623	37.549	-21.687	0.00	0.00	7
CA	SER	B	2	16.421	38.239	-22.955	0.00	0.00	6
CB	SER	B	2	14.966	38.166	-23.409	0.00	0.00	6
O	SER	B	2	14.690	39.185	-24.358	0.00	0.00	8
C	SER	B	2	16.826	39.705	-22.784	0.00	0.00	6
O	SER	B	2	16.722	40.242	-21.680	0.00	0.00	8
N	THR	B	2	17.273	40.344	-23.859	0.00	0.00	7
CA	THR	B	2	17.738	41.737	-23.762	0.00	0.00	6
CB	THR	B	2	19.260	41.759	-23.962	0.00	0.00	6
O	THR	B	2	19.868	41.092	-22.832	0.00	0.00	8
C	THR	B	2	19.889	43.137	-24.035	0.00	0.00	6
C	THR	B	2	16.962	42.631	-24.708	0.00	0.00	6
O	THR	B	2	17.285	43.792	-24.973	0.00	0.00	8
N	ARG	B	2	15.782	42.175	-25.133	0.00	0.00	7
CA	ARG	B	2	14.924	42.914	-26.051	0.00	0.00	6
CB	ARG	B	2	13.923	41.938	-26.690	0.00	0.00	6
C	ARG	B	2	13.305	42.435	-27.985	0.00	0.00	6
C	ARG	B	2	12.311	41.433	-28.553	0.00	0.00	6
N	ARG	B	2	12.906	40.609	-29.599	0.00	0.00	7
CZ	ARG	B	2	13.523	39.451	-29.399	0.00	0.00	6
N	ARG	B	2	13.642	38.939	-28.179	0.00	0.00	7
N	ARG	B	2	14.030	38.790	-30.433	0.00	0.00	7
C	ARG	B	2	14.195	44.087	-25.417	0.00	0.00	6
O	ARG	B	2	12.965	44.106	-25.333	0.00	0.00	8
N	ASN	B	2	14.906	45.140	-25.025	0.00	0.00	7
CA	ASN	B	2	14.339	46.315	-24.394	0.00	0.00	6
CB	ASN	B	2	15.448	47.195	-23.797	0.00	0.00	6
C	ASN	B	2	16.257	46.486	-22.732	0.00	0.00	6
O	ASN	B	2	15.799	46.299	-21.602	0.00	0.00	8
N	ASN	B	2	17.473	46.083	-23.082	0.00	0.00	7
C	ASN	B	2	13.481	47.176	-25.307	0.00	0.00	6
O	ASN	B	2	12.652	47.946	-24.811	0.00	0.00	8
N	ASP	B	2	13.641	47.077	-26.622	0.00	0.00	7
CA	ASP	B	2	12.853	47.865	-27.564	0.00	0.00	6
CB	ASP	B	2	13.411	47.770	-28.983	0.00	0.00	6
C	ASP	B	2	13.539	46.347	-29.487	0.00	0.00	6
O	ASP	B	2	14.477	45.642	-29.058	0.00	0.00	8
O	ASP	B	2	12.702	45.927	-30.313	0.00	0.00	8
C	ASP	B	2	11.388	47.443	-27.518	0.00	0.00	6
O	ASP	B	2	10.484	48.269	-27.634	0.00	0.00	8
N	ASN	B	2	11.153	46.153	-27.314	0.00	0.00	7
CA	ASN	B	2	9.811	45.601	-27.205	0.00	0.00	6
CB	ASN	B	2	9.387	45.031	-28.555	0.00	0.00	6
C	ASN	B	2	7.928	44.678	-28.693	0.00	0.00	6
O	ASN	B	2	7.470	44.389	-29.804	0.00	0.00	8
N	ASN	B	2	7.168	44.677	-27.605	0.00	0.00	7
C	ASN	B	2	9.750	44.542	-26.111	0.00	0.00	6
O	ASN	B	2	9.883	43.342	-26.353	0.00	0.00	8
N	PRO	B	2	9.509	44.976	-24.877	0.00	0.00	7
C	PRO	B	2	9.381	46.408	-24.497	0.00	0.00	6
CA	PRO	B	2	9.418	44.106	-23.722	0.00	0.00	6
CB	PRO	B	2	9.092	45.047	-22.564	0.00	0.00	6
C	PRO	B	2	9.566	46.386	-23.004	0.00	0.00	6
C	PRO	B	2	8.389	42.994	-23.813	0.00	0.00	6
O	PRO	B	2	8.645	41.874	-23.353	0.00	0.00	8
N	GLN	B	2	7.231	43.236	-24.419	0.00	0.00	7
CA	GLN	B	2	6.171	42.253	-24.546	0.00	0.00	6
CB	GLN	B	2	4.822	42.932	-24.816	0.00	0.00	6
C	GLN	B	2	4.330	43.835	-23.704	0.00	0.00	6
C	GLN	B	2	4.389	45.304	-24.073	0.00	0.00	6
O	GLN	B	2	5.374	45.778	-24.642	0.00	0.00	8
N	GLN	B	2	3.324	46.029	-23.745	0.00	0.00	7

Figure 1 - 36

CA	TYR	B	2	24.503	16.907	-17.311	0.00	0.00	6
CB	TYR	B	2	23.451	17.038	-18.431	0.00	0.00	6
C	TYR	B	2	24.048	17.513	-19.738	0.00	0.00	6
C	TYR	B	2	24.764	16.646	-20.552	0.00	0.00	6
CE	TYR	B	2	25.328	17.085	-21.735	0.00	0.00	6
C	TYR	B	2	23.920	18.836	-20.138	0.00	0.00	6
CE	TYR	B	2	24.481	19.285	-21.317	0.00	0.00	6
CZ	TYR	B	2	25.184	18.403	-22.110	0.00	0.00	6
O	TYR	B	2	25.745	18.844	-23.288	0.00	0.00	8
C	TYR	B	2	25.213	18.225	-17.058	0.00	0.00	6
O	TYR	B	2	26.443	18.260	-16.980	0.00	0.00	8
N	HIS	B	2	24.468	19.317	-16.925	0.00	0.00	7
CA	HIS	B	2	25.063	20.628	-16.677	0.00	0.00	6
CB	HIS	B	2	25.120	21.431	-17.973	0.00	0.00	6
C	HIS	B	2	25.949	22.675	-17.927	0.00	0.00	6
C	HIS	B	2	27.279	22.868	-18.087	0.00	0.00	6
N	HIS	B	2	25.406	23.923	-17.701	0.00	0.00	7
CE	HIS	B	2	26.363	24.831	-17.719	0.00	0.00	6
N	HIS	B	2	27.510	24.217	-17.952	0.00	0.00	7
C	HIS	B	2	24.288	21.375	-15.598	0.00	0.00	6
O	HIS	B	2	23.085	21.157	-15.436	0.00	0.00	8
N	MET	B	2	24.946	22.292	-14.889	0.00	0.00	7
CA	MET	B	2	24.297	23.020	-13.806	0.00	0.00	6
CB	MET	B	2	25.284	23.763	-12.915	0.00	0.00	6
C	MET	B	2	26.479	24.423	-13.565	0.00	0.00	6
SD	MET	B	2	27.340	25.556	-12.453	0.00	0.00	1
CE	MET	B	2	28.762	24.575	-11.990	0.00	0.00	6
C	MET	B	2	23.192	23.954	-14.283	0.00	0.00	6
O	MET	B	2	22.242	24.177	-13.521	0.00	0.00	8
N	THR	B	2	23.280	24.496	-15.491	0.00	0.00	7
CA	THR	B	2	22.249	25.396	-15.991	0.00	0.00	6
CB	THR	B	2	22.776	26.836	-16.144	0.00	0.00	6
O	THR	B	2	24.147	26.806	-16.565	0.00	0.00	8
C	THR	B	2	22.665	27.584	-14.824	0.00	0.00	6
C	THR	B	2	21.657	24.943	-17.318	0.00	0.00	6
O	THR	B	2	20.454	25.103	-17.539	0.00	0.00	8
N	SER	B	2	22.480	24.384	-18.196	0.00	0.00	7
CA	SER	B	2	22.012	23.923	-19.495	0.00	0.00	6
CB	SER	B	2	23.128	24.054	-20.538	0.00	0.00	6
O	SER	B	2	23.448	25.410	-20.790	0.00	0.00	8
C	SER	B	2	21.533	22.477	-19.459	0.00	0.00	6
O	SER	B	2	22.118	21.612	-18.811	0.00	0.00	8
N	PRO	B	2	20.485	22.196	-20.221	0.00	0.00	7
C	PRO	B	2	19.715	23.172	-21.033	0.00	0.00	6
CA	PRO	B	2	19.932	20.860	-20.357	0.00	0.00	6
CB	PRO	B	2	18.460	21.148	-20.623	0.00	0.00	6
C	PRO	B	2	18.445	22.437	-21.365	0.00	0.00	6
C	PRO	B	2	20.565	20.112	-21.518	0.00	0.00	6
O	PRO	B	2	21.197	20.714	-22.390	0.00	0.00	8
N	PRO	B	2	20.414	18.795	-21.539	0.00	0.00	7
C	PRO	B	2	19.641	18.000	-20.560	0.00	0.00	6
CA	PRO	B	2	20.896	17.984	-22.643	0.00	0.00	6
CB	PRO	B	2	20.726	16.551	-22.173	0.00	0.00	6
C	PRO	B	2	19.915	16.576	-20.935	0.00	0.00	6
C	PRO	B	2	20.079	18.275	-23.889	0.00	0.00	6
O	PRO	B	2	18.844	18.264	-23.831	0.00	0.00	8
N	GLU	B	2	20.721	18.449	-25.038	0.00	0.00	7
CA	GLU	B	2	20.025	18.704	-26.299	0.00	0.00	6
CB	GLU	B	2	21.031	18.855	-27.441	0.00	0.00	6
C	GLU	B	2	22.096	19.912	-27.188	0.00	0.00	6
C	GLU	B	2	22.372	20.788	-28.392	0.00	0.00	6
O	GLU	B	2	23.395	20.565	-29.075	0.00	0.00	8
O	GLU	B	2	21.570	21.707	-28.665	0.00	0.00	8
C	GLU	B	2	18.991	17.627	-26.599	0.00	0.00	6

O	GLU	B	2	17.914	17.862	-27.146	0.00	0.00	8
N	ASN	B	2	19.270	16.400	-26.211	0.00	0.00	7
CA	ASN	B	2	18.435	15.232	-26.207	0.00	0.00	6
CB	ASN	B	2	19.172	14.173	-25.349	0.00	0.00	6
C	ASN	B	2	18.845	12.748	-25.717	0.00	0.00	6
O	ASN	B	2	19.753	11.936	-25.906	0.00	0.00	8
N	ASN	B	2	17.563	12.424	-25.817	0.00	0.00	7
C	ASN	B	2	17.071	15.424	-25.550	0.00	0.00	6
O	ASN	B	2	16.066	14.871	-25.996	0.00	0.00	8
N	GLY	B	2	17.065	16.049	-24.372	0.00	0.00	7
CA	GLY	B	2	15.866	16.222	-23.566	0.00	0.00	6
C	GLY	B	2	15.598	14.984	-22.712	0.00	0.00	6
O	GLY	B	2	14.492	14.758	-22.223	0.00	0.00	8
N	ALA	B	2	16.622	14.173	-22.501	0.00	0.00	7
CA	ALA	B	2	16.575	12.927	-21.771	0.00	0.00	6
CB	ALA	B	2	17.997	12.361	-21.662	0.00	0.00	6
C	ALA	B	2	15.955	12.959	-20.385	0.00	0.00	6
O	ALA	B	2	15.249	12.014	-20.012	0.00	0.00	8
N	GLY	B	2	16.284	13.950	-19.564	0.00	0.00	7
CA	GLY	B	2	15.732	14.032	-18.215	0.00	0.00	6
C	GLY	B	2	14.264	14.437	-18.254	0.00	0.00	6
O	GLY	B	2	13.456	13.967	-17.452	0.00	0.00	8
N	ALA	B	2	13.921	15.313	-19.193	0.00	0.00	7
CA	ALA	B	2	12.549	15.782	-19.358	0.00	0.00	6
CB	ALA	B	2	12.508	16.914	-20.373	0.00	0.00	6
C	ALA	B	2	11.638	14.633	-19.775	0.00	0.00	6
O	ALA	B	2	10.537	14.466	-19.251	0.00	0.00	8
N	ALA	B	2	12.125	13.781	-20.672	0.00	0.00	7
CA	ALA	B	2	11.409	12.585	-21.094	0.00	0.00	6
CB	ALA	B	2	12.212	11.839	-22.151	0.00	0.00	6
C	ALA	B	2	11.158	11.665	-19.904	0.00	0.00	6
O	ALA	B	2	10.040	11.206	-19.674	0.00	0.00	8
N	LEU	B	2	12.207	11.418	-19.123	0.00	0.00	7
CA	LEU	B	2	12.127	10.568	-17.944	0.00	0.00	6
CB	LEU	B	2	13.483	10.549	-17.234	0.00	0.00	6
C	LEU	B	2	14.093	9.186	-16.906	0.00	0.00	6
C	LEU	B	2	15.393	9.365	-16.133	0.00	0.00	6
C	LEU	B	2	13.122	8.312	-16.125	0.00	0.00	6
C	LEU	B	2	11.044	11.001	-16.966	0.00	0.00	6
O	LEU	B	2	10.249	10.182	-16.499	0.00	0.00	8
N	ALA	B	2	10.992	12.293	-16.648	0.00	0.00	7
CA	ALA	B	2	9.989	12.831	-15.736	0.00	0.00	6
CB	ALA	B	2	10.311	14.279	-15.395	0.00	0.00	6
C	ALA	B	2	8.580	12.703	-16.305	0.00	0.00	6
O	ALA	B	2	7.642	12.413	-15.555	0.00	0.00	8
N	MET	B	2	8.424	12.909	-17.614	0.00	0.00	7
CA	MET	B	2	7.111	12.712	-18.239	0.00	0.00	6
CB	MET	B	2	7.060	13.311	-19.636	0.00	0.00	6
C	MET	B	2	7.126	14.834	-19.637	0.00	0.00	6
SD	MET	B	2	6.856	15.558	-21.262	0.00	0.00	1
CE	MET	B	2	8.526	15.634	-21.899	0.00	0.00	6
C	MET	B	2	6.802	11.220	-18.214	0.00	0.00	6
O	MET	B	2	5.763	10.790	-17.711	0.00	0.00	8
N	ALA	B	2	7.773	10.402	-18.613	0.00	0.00	7
CA	ALA	B	2	7.647	8.952	-18.540	0.00	0.00	6
CB	ALA	B	2	8.954	8.281	-18.938	0.00	0.00	6
C	ALA	B	2	7.235	8.493	-17.145	0.00	0.00	6
O	ALA	B	2	6.285	7.716	-17.030	0.00	0.00	8
N	ASN	B	2	7.901	8.968	-16.094	0.00	0.00	7
CA	ASN	B	2	7.583	8.566	-14.733	0.00	0.00	6
CB	ASN	B	2	8.627	9.075	-13.730	0.00	0.00	6
C	ASN	B	2	9.949	8.343	-13.851	0.00	0.00	6
O	ASN	B	2	9.990	7.167	-14.216	0.00	0.00	8
N	ASN	B	2	11.042	9.034	-13.551	0.00	0.00	7

Figure 1 - 40

O	GLU	B	3	-8.326	15.026	-17.565	0.00	0.00	8
N	TYR	B	3	-7.171	14.764	-19.474	0.00	0.00	7
CA	TYR	B	3	-5.872	14.836	-18.820	0.00	0.00	6
CB	TYR	B	3	-5.066	13.550	-19.063	0.00	0.00	6
C	TYR	B	3	-5.646	12.321	-18.401	0.00	0.00	6
C	TYR	B	3	-6.417	11.425	-19.132	0.00	0.00	6
CE	TYR	B	3	-6.978	10.312	-18.535	0.00	0.00	6
C	TYR	B	3	-5.454	12.071	-17.051	0.00	0.00	6
CE	TYR	B	3	-6.009	10.959	-16.445	0.00	0.00	6
CZ	TYR	B	3	-6.769	10.085	-17.192	0.00	0.00	6
O	TYR	B	3	-7.326	8.976	-16.597	0.00	0.00	8
C	TYR	B	3	-5.034	16.018	-19.294	0.00	0.00	6
O	TYR	B	3	-5.017	16.342	-20.482	0.00	0.00	8
N	THR	B	3	-4.282	16.626	-18.381	0.00	0.00	7
CA	THR	B	3	-3.292	17.636	-18.718	0.00	0.00	6
CB	THR	B	3	-3.692	19.082	-18.388	0.00	0.00	6
O	THR	B	3	-4.186	19.170	-17.044	0.00	0.00	8
C	THR	B	3	-4.736	19.619	-19.354	0.00	0.00	6
C	THR	B	3	-1.972	17.344	-17.995	0.00	0.00	6
O	THR	B	3	-1.947	16.819	-16.887	0.00	0.00	8
N	LEU	B	3	-0.873	17.725	-18.626	0.00	0.00	7
CA	LEU	B	3	0.473	17.536	-18.101	0.00	0.00	6
CB	LEU	B	3	1.262	16.734	-19.134	0.00	0.00	6
C	LEU	B	3	2.652	16.201	-18.820	0.00	0.00	6
C	LEU	B	3	2.591	14.952	-17.955	0.00	0.00	6
C	LEU	B	3	3.405	15.888	-20.110	0.00	0.00	6
C	LEU	B	3	1.144	18.878	-17.835	0.00	0.00	6
O	LEU	B	3	1.190	19.712	-18.745	0.00	0.00	8
N	CYS	B	3	1.623	19.127	-16.616	0.00	0.00	7
CA	CYS	B	3	2.341	20.362	-16.319	0.00	0.00	6
CB	CYS	B	3	1.761	21.154	-15.146	0.00	0.00	6
SG	CYS	B	3	2.784	22.605	-14.750	0.00	0.00	1
C	CYS	B	3	3.817	20.081	-16.038	0.00	0.00	6
O	CYS	B	3	4.172	19.382	-15.093	0.00	0.00	8
N	ASN	B	3	4.681	20.666	-16.852	0.00	0.00	7
CA	ASN	B	3	6.113	20.457	-16.801	0.00	0.00	6
CB	ASN	B	3	6.561	20.213	-18.260	0.00	0.00	6
C	ASN	B	3	6.424	18.773	-18.697	0.00	0.00	6
O	ASN	B	3	6.208	17.872	-17.887	0.00	0.00	8
N	ASN	B	3	6.574	18.544	-19.997	0.00	0.00	7
C	ASN	B	3	6.977	21.568	-16.233	0.00	0.00	6
O	ASN	B	3	6.881	22.730	-16.617	0.00	0.00	8
N	SER	B	3	7.954	21.187	-15.413	0.00	0.00	7
CA	SER	B	3	8.937	22.105	-14.851	0.00	0.00	6
CB	SER	B	3	8.579	22.503	-13.422	0.00	0.00	6
O	SER	B	3	8.046	23.810	-13.359	0.00	0.00	8
C	SER	B	3	10.315	21.445	-14.860	0.00	0.00	6
O	SER	B	3	10.513	20.427	-14.194	0.00	0.00	8
N	PHE	B	3	11.238	21.977	-15.649	0.00		

CA	PHE	B	4	18.387	24.746	-12.897	0.00	0.00	6
CB	PHE	B	4	18.720	26.141	-12.373	0.00	0.00	6
C	PHE	B	4	18.292	27.221	-13.330	0.00	0.00	6
C	PHE	B	4	17.267	28.087	-13.002	0.00	0.00	6
C	PHE	B	4	18.916	27.368	-14.558	0.00	0.00	6
CE	PHE	B	4	16.866	29.079	-13.876	0.00	0.00	6
CE	PHE	B	4	18.522	28.357	-15.436	0.00	0.00	6
CZ	PHE	B	4	17.495	29.215	-15.095	0.00	0.00	6
C	PHE	B	4	18.862	23.638	-11.971	0.00	0.00	6
O	PHE	B	4	18.146	23.237	-11.054	0.00	0.00	8
N	GLY	B	4	20.035	23.085	-12.261	0.00	0.00	7
CA	GLY	B	4	20.579	21.974	-11.489	0.00	0.00	6
C	GLY	B	4	20.138	20.638	-12.082	0.00	0.00	6
O	GLY	B	4	20.442	19.568	-11.554	0.00	0.00	8
N	GLY	B	4	19.372	20.671	-13.162	0.00	0.00	7
CA	GLY	B	4	18.843	19.509	-13.835	0.00	0.00	6
C	GLY	B	4	17.780	18.774	-13.036	0.00	0.00	6
O	GLY	B	4	17.658	17.555	-13.171	0.00	0.00	8
N	THR	B	4	16.986	19.478	-12.237	0.00	0.00	7
CA	THR	B	4	15.949	18.817	-11.440	0.00	0.00	6
CB	THR	B	4	15.976	19.325	-9.993	0.00	0.00	6
O	THR	B	4	14.911	18.730	-9.243	0.00	0.00	8
C	THR	B	4	15.873	20.840	-9.915	0.00	0.00	6
C	THR	B	4	14.607	18.975	-12.134	0.00	0.00	6
O	THR	B	4	14.143	20.085	-12.401	0.00	0.00	8
N	ASN	B	4	14.012	17.851	-12.542	0.00	0.00	7
CA	ASN	B	4	12.791	17.853	-13.322	0.00	0.00	6
CB	ASN	B	4	12.936	16.993	-14.591	0.00	0.00	6
C	ASN	B	4	14.167	17.308	-15.404	0.00	0.00	6
O	ASN	B	4	14.327	18.432	-15.878	0.00	0.00	8
N	ASN	B	4	15.033	16.317	-15.556	0.00	0.00	7
C	ASN	B	4	11.564	17.303	-12.604	0.00	0.00	6
O	ASN	B	4	11.653	16.434	-11.745	0.00	0.00	8
N	GLY	B	4	10.405	17.769	-13.071	0.00	0.00	7
CA	GLY	B	4	9.142	17.309	-12.516	0.00	0.00	6
C	GLY	B	4	7.990	17.509	-13.491	0.00	0.00	6
O	GLY	B	4	7.993	18.405	-14.327	0.00	0.00	8
N	SER	B	4	6.987	16.650	-13.367	0.00	0.00	7
CA	SER	B	4	5.782	16.715	-14.170	0.00	0.00	6
CB	SER	B	4	5.822	15.765	-15.365	0.00	0.00	6
O	SER	B	4	6.920	15.961	-16.224	0.00	0.00	8
C	SER	B	4	4.581	16.334	-13.302	0.00	0.00	6
O	SER	B	4	4.688	15.411	-12.495	0.00	0.00	8
N	LEU	B	4	3.471	17.032	-13.484	0.00	0.00	7
CA	LEU	B	4	2.249	16.710	-12.751	0.00	0.00	6
CB	LEU	B	4	1.830	17.338	-11.819	0.00	0.00	6
C	LEU	B	4	2.585	17.940	-10.488	0.00	0.00	6
C	LEU	B	4	2.403	19.314	-9.863	0.00	0.00	6
C	LEU	B	4	2.137	16.855	-9.521	0.00	0.00	6
C	LEU	B	4	1.166	16.376	-13.777	0.00	0.00	6
O	LEU	B	4	1.216	16.876	-14.906	0.00	0.00	8
N	ILE	B	4	0.306	15.412	-13.474	0.00	0.00	7
CA	ILE	B	4	-0.784	15.030	-14.359	0.00	0.00	6
CB	ILE	B	4	-0.723	13.580	-14.866	0.00	0.00	6
C	ILE	B	4	-2.009	13.208	-15.599	0.00	0.00	6
C	ILE	B	4	0.471	13.365	-15.798	0.00	0.00	6
C	ILE	B	4	0.661	11.935	-16.250	0.00	0.00	6
C	ILE	B	4	-2.112	15.245	-13.630	0.00	0.00	6
O	ILE	B	4	-2.303	14.764	-12.516	0.00	0.00	8
N	PHE	B	4	-3.015	15.973	-14.279	0.00	0.00	7
CA	PHE	B	4	-4.320	16.257	-13.690	0.00	0.00	6
CB	PHE	B	4	-4.534	17.768	-13.596	0.00	0.00	6
C	PHE	B	4	-3.628	18.449	-12.608	0.00	0.00	6
C	PHE	B	4	-2.421	18.992	-13.015	0.00	0.00	6

Figure 1 - 47

C	PHE	B	4	-3.974	18.529	-11.268	0.00	0.00	6
CE	PHE	B	4	-1.583	19.615	-12.109	0.00	0.00	6
CE	PHE	B	4	-3.142	19.154	-10.360	0.00	0.00	6
CZ	PHE	B	4	-1.948	19.701	-10.780	0.00	0.00	6
C	PHE	B	4	-5.433	15.582	-14.484	0.00	0.00	6
O	PHE	B	4	-5.299	15.351	-15.685	0.00	0.00	8
N	LYS	B	4	-6.508	15.211	-13.796	0.00	0.00	7
CA	LYS	B	4	-7.621	14.523	-14.445	0.00	0.00	6
CB	LYS	B	4	-7.615	13.048	-14.064	0.00	0.00	6
C	LYS	B	4	-8.945	12.390	-13.771	0.00	0.00	6
C	LYS	B	4	-9.066	11.022	-14.425	0.00	0.00	6
CE	LYS	B	4	-9.980	10.113	-13.620	0.00	0.00	6
NZ	LYS	B	4	-11.257	10.787	-13.251	0.00	0.00	7
C	LYS	B	4	-8.942	15.210	-14.115	0.00	0.00	6
O	LYS	B	4	-9.212	15.563	-12.970	0.00	0.00	8
N	LYS	B	4	-9.765	15.394	-15.142	0.00	0.00	7
CA	LYS	B	4	-11.067	16.029	-14.990	0.00	0.00	6
CB	LYS	B	4	-11.634	16.391	-16.366	0.00	0.00	6
C	LYS	B	4	-12.465	17.660	-16.399	0.00	0.00	6
C	LYS	B	4	-13.928	17.380	-16.089	0.00	0.00	6
CE	LYS	B	4	-14.796	18.590	-16.391	0.00	0.00	6
NZ	LYS	B	4	-14.788	19.577	-15.277	0.00	0.00	7
C	LYS	B	4	-12.043	15.106	-14.269	0.00	0.00	6
O	LYS	B	4	-12.185	13.944	-14.652	0.00	0.00	8
N	ILE	B	4	-12.698	15.610	-13.230	0.00	0.00	7
CA	ILE	B	4	-13.715	14.833	-12.522	0.00	0.00	6
CB	ILE	B	4	-13.357	14.578	-11.053	0.00	0.00	6
C	ILE	B	4	-14.584	14.417	-10.163	0.00	0.00	6
C	ILE	B	4	-12.478	13.322	-10.945	0.00	0.00	6
C	ILE	B	4	-11.906	13.091	-9.564	0.00	0.00	6
C	ILE	B	4	-15.060	15.546	-12.659	0.00	0.00	6
O	ILE	B	4	-15.481	15.769	-13.816	0.00	0.00	8
O1	WAT	W	5	4.504	27.399	-19.536	0.00	0.00	8
O1	WAT	W	5	7.437	28.629	2.535	0.00	0.00	8
O1	WAT	W	5	14.567	39.281	-19.752	0.00	0.00	8
O1	WAT	W	5	12.567	39.856	-2.839	0.00	0.00	8
O1	WAT	W	5	12.015	35.396	-4.390	0.00	0.00	8
O1	WAT	W	5	3.319	30.612	-17.061	0.00	0.00	8
O1	WAT	W	5	16.094	26.918	-5.435	0.00	0.00	8
O1	WAT	W	5	8.209	39.238	-23.056	0.00	0.00	8
O1	WAT	W	5	18.807	20.357	-7.960	0.00	0.00	8
O1	WAT	W	5	-13.395	21.538	1.565	0.00	0.00	8
O1	WAT	W	5	24.930	41.412	-15.101	0.00	0.00	8
O1	WAT	W	5	21.290	38.294	-20.198	0.00	0.00	8
O1	WAT	W	5	15.902	50.395	9.343	0.00	0.00	8
O1	WAT	W	5	-2.782	8.166	-8.701	0.00	0.00	8
O1	WAT	W	5	18.738	27.340	-19.439	0.00	0.00	8
O1	WAT	W	5	-1.747	11.046	-6.351	0.00	0.00	8
O1	WAT	W	5	6.680	14.967	-34.855	0.00	0.00	8
O1	WAT	W	5	22.057	48.723	-9.374	0.00	0.00	8
O1	WAT	W	5	-6.611	39.165	-2.117	0.00	0.00	8
O1	WAT	W	5	13.624	8.609	-12.588	0.00	0.00	8
O1	WAT	W	5	9.255	7.220	-29.727	0.00	0.00	8
O1	WAT	W	5	-5.734	12.781	-26.436	0.00	0.00	8
O1	WAT	W	5	21.680	48.304	-5.494	0.00	0.00	8
O1	WAT	W	5	15.561	45.821	-2.731	0.00	0.00	8
O1	WAT	W	5	0.642	10.760	10.232	0.00	0.00	8
O1	WAT	W	5	0.990	48.249	1.863	0.00	0.00	8
O1	WAT	W	5	20.915	17.564	-30.457	0.00	0.00	8
O1	WAT	W	5	16.863	23.110	-17.142	0.00	0.00	8
O1	WAT	W	5	9.631	43.771	-32.080	0.00	0.00	8
O1	WAT	W	5	-9.127	0.966	-13.608	0.00	0.00	8
O1	WAT	W	5	23.605	12.660	-18.246	0.00	0.00	8

Figure 1 - 48

N	LYS	A	2	5.691	-3.942	0.967	1.00	59.01	N
CA	LYS	A	2	6.181	-2.836	1.843	1.00	59.40	C
C	LYS	A	2	7.698	-2.690	1.729	1.00	58.26	C
O	LYS	A	2	8.433	-3.674	1.800	1.00	58.76	O
CB	LYS	A	2	5.769	-3.035	3.298	1.00	59.99	C
CG	LYS	A	2	6.542	-2.171	4.281	1.00	60.75	C
CD	LYS	A	2	5.621	-1.406	5.211	1.00	61.69	C
CE	LYS	A	2	5.333	-0.004	4.701	1.00	62.26	C
NZ	LYS	A	2	5.569	1.027	5.757	1.00	62.54	N
N	ARG	A	3	8.164	-1.457	1.572	1.00	56.23	N
CA	ARG	A	3	9.587	-1.211	1.400	1.00	54.46	C
C	ARG	A	3	10.254	-0.621	2.629	1.00	53.07	C
O	ARG	A	3	9.908	0.442	3.142	1.00	53.04	O
CB	ARG	A	3	9.797	-0.330	0.163	1.00	54.51	C
CG	ARG	A	3	9.528	-1.088	-1.137	1.00	54.53	C
CD	ARG	A	3	9.198	-0.128	-2.267	1.00	54.58	C
NE	ARG	A	3	10.369	0.430	-2.917	1.00	54.17	N
CZ	ARG	A	3	11.239	-0.232	-3.660	1.00	54.41	C
NH1	ARG	A	3	11.105	-1.535	-3.867	1.00	54.22	N
NH2	ARG	A	3	12.268	0.409	-4.208	1.00	55.03	N
N	ARG	A	4	11.255	-1.351	3.116	1.00	51.11	N
CA	ARG	A	4	12.014	-0.957	4.293	1.00	49.31	C
C	ARG	A	4	13.305	-0.261	3.888	1.00	46.70	C
O	ARG	A	4	14.075	-0.757	3.065	1.00	45.87	O
CB	ARG	A	4	12.313	-2.184	5.161	1.00	51.04	C
CG	ARG	A	4	11.082	-3.026	5.462	1.00	52.54	C
CD	ARG	A	4	11.310	-4.014	6.588	1.00	54.18	C
NE	ARG	A	4	12.714	-4.381	6.740	1.00	55.76	N
CZ	ARG	A	4	13.204	-5.089	7.754	1.00	55.81	C
NH1	ARG	A	4	12.388	-5.510	8.707	1.00	56.21	N
NH2	ARG	A	4	14.499	-5.363	7.792	1.00	56.00	N
N	VAL	A	5	13.512	0.929	4.436	1.00	44.00	N
CA	VAL	A	5	14.691	1.721	4.082	1.00	41.65	C
C	VAL	A	5	15.765	1.553	5.144	1.00	40.39	C
O	VAL	A	5	15.466	1.605	6.342	1.00	40.29	O
CB	VAL	A	5	14.334	3.204	3.904	1.00	41.18	C
CG1	VAL	A	5	15.542	4.022	3.494	1.00	40.93	C
CG2	VAL	A	5	13.215	3.337	2.878	1.00	40.99	C
N	VAL	A	6	16.989	1.323	4.687	1.00	38.36	N
CA	VAL	A	6	18.127	1.134	5.579	1.00	36.46	C
C	VAL	A	6	19.270	2.069	5.204	1.00	35.96	C
O	VAL	A	6	19.367	2.549	4.078	1.00	34.89	O
CB	VAL	A	6	18.597	-0.331	5.583	1.00	36.36	C
CG1	VAL	A	6	17.633	-1.212	6.377	1.00	35.25	C
CG2	VAL	A	6	18.774	-0.883	4.176	1.00	34.82	C
N	VAL	A	7	20.114	2.404	6.175	1.00	36.29	N
CA	VAL	A	7	21.209	3.359	5.973	1.00	34.89	C
C	VAL	A	7	22.508	2.606	5.723	1.00	35.21	C
O	VAL	A	7	23.107	2.026	6.633	1.00	34.55	O
CB	VAL	A	7	21.352	4.266	7.205	1.00	34.25	C
CG1	VAL	A	7	22.435	5.308	6.974	1.00	34.66	C
CG2	VAL	A	7	20.030	4.915	7.568	1.00	32.51	C
N	THR	A	8	22.947	2.600	4.468	1.00	35.16	N
CA	THR	A	8	24.151	1.902	4.077	1.00	34.77	C
C	THR	A	8	25.366	2.768	3.841	1.00	34.34	C
O	THR	A	8	26.312	2.285	3.191	1.00	35.61	O
CB	THR	A	8	23.893	1.120	2.751	1.00	35.46	C
OG1	THR	A	8	23.765	2.081	1.693	1.00	35.07	O
CG2	THR	A	8	22.666	0.247	2.872	1.00	34.29	C
N	GLY	A	9	25.403	4.010	4.292	1.00	33.53	N
CA	GLY	A	9	26.572	4.846	4.008	1.00	32.71	C
C	GLY	A	9	26.496	6.173	4.745	1.00	32.55	C
O	GLY	A	9	25.472	6.847	4.718	1.00	32.58	O

Figure 2-1

N	LEU	A	10	27.591	6.534	5.404	1.00	31.65	N
CA	LEU	A	10	27.691	7.753	6.182	1.00	30.79	C
C	LEU	A	10	28.815	8.653	5.700	1.00	30.11	C
O	LEU	A	10	29.837	8.168	5.209	1.00	30.41	O
CB	LEU	A	10	27.912	7.374	7.657	1.00	31.04	C
CG	LEU	A	10	26.798	6.560	8.320	1.00	31.18	C
CD1	LEU	A	10	27.208	6.161	9.736	1.00	31.32	C
CD2	LEU	A	10	25.488	7.329	8.323	1.00	30.03	C
N	GLY	A	11	28.643	9.963	5.814	1.00	29.43	N
CA	GLY	A	11	29.679	10.911	5.372	1.00	28.90	C
C	GLY	A	11	29.509	12.228	6.120	1.00	28.84	C
O	GLY	A	11	28.368	12.646	6.360	1.00	27.25	O
N	MET	A	12	30.616	12.889	6.517	1.00	29.01	N
CA	MET	A	12	30.376	14.128	7.269	1.00	29.71	C
C	MET	A	12	31.538	15.041	7.553	1.00	29.99	C
O	MET	A	12	32.635	14.675	7.959	1.00	30.94	O
CB	MET	A	12	29.709	13.689	8.579	1.00	30.44	C
CG	MET	A	12	30.111	14.370	9.851	1.00	31.28	C
SD	MET	A	12	29.114	13.787	11.236	1.00	33.04	S
CE	MET	A	12	29.030	15.291	12.208	1.00	34.14	C
N	LEU	A	13	31.255	16.339	7.480	1.00	29.20	N
CA	LEU	A	13	32.186	17.389	7.856	1.00	28.50	C
C	LEU	A	13	31.557	18.111	9.057	1.00	28.52	C
O	LEU	A	13	30.355	18.378	9.039	1.00	28.74	O
CB	LEU	A	13	32.394	18.402	6.750	1.00	28.65	C
CG	LEU	A	13	33.435	18.122	5.680	1.00	28.65	C
CD1	LEU	A	13	33.357	19.187	4.601	1.00	28.55	C
CD2	LEU	A	13	34.829	18.057	6.293	1.00	28.84	C
N	SER	A	14	32.344	18.403	10.070	1.00	28.97	N
CA	SER	A	14	31.799	19.072	11.255	1.00	28.21	C
C	SER	A	14	32.909	19.787	12.004	1.00	27.92	C
O	SER	A	14	34.097	19.551	11.780	1.00	28.19	O
CB	SER	A	14	31.141	18.044	12.170	1.00	28.44	C
OG	SER	A	14	32.052	17.670	13.191	1.00	29.39	O
N	PRO	A	15	32.515	20.647	12.923	1.00	27.64	N
CA	PRO	A	15	33.437	21.428	13.717	1.00	28.13	C
C	PRO	A	15	34.385	20.619	14.582	1.00	28.10	C
O	PRO	A	15	35.465	21.116	14.931	1.00	26.91	O
CB	PRO	A	15	32.536	22.318	14.571	1.00	28.32	C
CG	PRO	A	15	31.220	22.323	13.885	1.00	28.67	C
CD	PRO	A	15	31.096	20.981	13.207	1.00	27.90	C
N	VAL	A	16	34.019	19.402	14.975	1.00	28.38	N
CA	VAL	A	16	34.884	18.572	15.791	1.00	28.90	C
C	VAL	A	16	35.607	17.534	14.941	1.00	29.97	C
O	VAL	A	16	36.453	16.796	15.472	1.00	31.83	O
CB	VAL	A	16	34.157	17.879	16.955	1.00	28.71	C
CG1	VAL	A	16	33.534	18.907	17.896	1.00	29.04	C
CG2	VAL	A	16	33.097	16.901	16.489	1.00	28.08	C
N	GLY	A	17	35.307	17.450	13.648	1.00	29.27	N
CA	GLY	A	17	35.990	16.446	12.835	1.00	30.51	C
C	GLY	A	17	35.651	16.531	11.360	1.00	31.65	C
O	GLY	A	17	34.569	16.998	10.992	1.00	32.81	O
N	ASN	A	18	36.559	16.075	10.506	1.00	31.30	N
CA	ASN	A	18	36.365	16.100	9.062	1.00	30.77	C
C	ASN	A	18	35.892	14.767	8.528	1.00	29.51	C
O	ASN	A	18	35.733	14.560	7.319	1.00	29.78	O
CB	ASN	A	18	37.678	16.530	8.381	1.00	32.68	C
CG	ASN	A	18	37.873	18.028	8.512	1.00	35.49	C
OD1	ASN	A	18	36.915	18.750	8.815	1.00	37.19	O
ND2	ASN	A	18	39.081	18.526	8.303	1.00	36.58	N
N	THR	A	19	35.804	13.749	9.379	1.00	27.98	N
CA	THR	A	19	35.289	12.456	8.960	1.00	27.30	C
C	THR	A	19	34.258	11.975	9.989	1.00	27.68	C

Figure 2-2

O	THR	A	19	34.070	12.579	11.046	1.00	28.33	O
CB	THR	A	19	36.328	11.346	8.760	1.00	25.95	C
OG1	THR	A	19	36.898	10.987	10.030	1.00	26.38	O
CG2	THR	A	19	37.418	11.733	7.792	1.00	23.99	C
N	VAL	A	20	33.560	10.909	9.640	1.00	27.75	N
CA	VAL	A	20	32.537	10.396	10.550	1.00	28.58	C
C	VAL	A	20	33.159	9.898	11.840	1.00	30.09	C
O	VAL	A	20	32.870	10.399	12.926	1.00	31.00	O
CB	VAL	A	20	31.737	9.270	9.872	1.00	27.71	C
CG1	VAL	A	20	30.836	8.588	10.881	1.00	28.09	C
CG2	VAL	A	20	30.975	9.838	8.685	1.00	26.96	C
N	GLU	A	21	34.033	8.897	11.735	1.00	31.53	N
CA	GLU	A	21	34.669	8.328	12.915	1.00	32.01	C
C	GLU	A	21	35.385	9.347	13.770	1.00	32.56	C
O	GLU	A	21	35.216	9.306	15.005	1.00	33.46	O
CB	GLU	A	21	35.592	7.178	12.500	1.00	32.25	C
CG	GLU	A	21	34.828	6.028	11.845	1.00	32.20	C
CD	GLU	A	21	33.779	5.403	12.731	1.00	32.65	C
OE1	GLU	A	21	33.806	5.603	13.972	1.00	33.29	O
OE2	GLU	A	21	32.893	4.693	12.198	1.00	32.86	O
N	SER	A	22	36.124	10.300	13.198	1.00	32.24	N
CA	SER	A	22	36.864	11.236	14.055	1.00	31.95	C
C	SER	A	22	35.894	12.051	14.892	1.00	32.52	C
O	SER	A	22	36.024	12.198	16.107	1.00	33.65	O
CB	SER	A	22	37.774	12.135	13.245	1.00	32.45	C
OG	SER	A	22	37.164	12.619	12.073	1.00	33.99	O
N	THR	A	23	34.883	12.592	14.222	1.00	32.30	N
CA	THR	A	23	33.842	13.388	14.853	1.00	30.89	C
C	THR	A	23	33.219	12.640	16.017	1.00	30.74	C
O	THR	A	23	33.074	13.176	17.109	1.00	30.91	O
CB	THR	A	23	32.754	13.699	13.800	1.00	30.18	C
OG1	THR	A	23	33.375	14.516	12.799	1.00	30.03	O
CG2	THR	A	23	31.561	14.400	14.404	1.00	29.43	C
N	TRP	A	24	32.834	11.394	15.770	1.00	30.66	N
CA	TRP	A	24	32.248	10.519	16.775	1.00	31.12	C
C	TRP	A	24	33.139	10.322	17.989	1.00	31.58	C
O	TRP	A	24	32.633	10.269	19.117	1.00	32.40	O
CB	TRP	A	24	31.898	9.174	16.126	1.00	30.43	C
CG	TRP	A	24	31.118	8.241	16.993	1.00	29.54	C
CD1	TRP	A	24	31.407	6.936	17.273	1.00	29.43	C
CD2	TRP	A	24	29.913	8.537	17.709	1.00	29.07	C
NE1	TRP	A	24	30.455	6.403	18.106	1.00	29.04	N
CE2	TRP	A	24	29.526	7.366	18.388	1.00	28.68	C
CE3	TRP	A	24	29.120	9.680	17.823	1.00	28.43	C
CZ2	TRP	A	24	28.382	7.304	19.175	1.00	28.30	C
CZ3	TRP	A	24	27.982	9.609	18.599	1.00	28.58	C
CH2	TRP	A	24	27.623	8.433	19.274	1.00	28.30	C
N	LYS	A	25	34.456	10.210	17.816	1.00	32.36	N
CA	LYS	A	25	35.365	10.069	18.950	1.00	32.47	C
C	LYS	A	25	35.384	11.367	19.753	1.00	31.77	C
O	LYS	A	25	35.161	11.344	20.966	1.00	32.00	O
CB	LYS	A	25	36.786	9.706	18.533	1.00	34.20	C
CG	LYS	A	25	36.856	8.568	17.532	1.00	36.79	C
CD	LYS	A	25	38.162	7.795	17.623	1.00	38.74	C
CE	LYS	A	25	38.112	6.579	16.685	1.00	39.99	C
NZ	LYS	A	25	39.171	5.589	17.053	1.00	40.83	N
N	ALA	A	26	35.488	12.495	19.055	1.00	30.32	N
CA	ALA	A	26	35.467	13.791	19.718	1.00	29.97	C
C	ALA	A	26	34.201	14.001	20.527	1.00	30.40	C
O	ALA	A	26	34.274	14.526	21.654	1.00	31.66	O
CB	ALA	A	26	35.654	14.915	18.714	1.00	30.12	C
N	LEU	A	27	33.043	13.626	19.995	1.00	30.16	N
CA	LEU	A	27	31.798	13.797	20.745	1.00	30.85	C

Figure 2-3

C	LEU	A	27	31.799	12.936	22.006	1.00	31.50	C
O	LEU	A	27	31.470	13.405	23.098	1.00	31.92	O
CB	LEU	A	27	30.585	13.468	19.896	1.00	30.80	C
CG	LEU	A	27	30.244	14.307	18.673	1.00	30.36	C
CD1	LEU	A	27	28.797	14.053	18.270	1.00	30.28	C
CD2	LEU	A	27	30.456	15.790	18.910	1.00	30.98	C
N	LEU	A	28	32.181	11.666	21.869	1.00	31.46	N
CA	LEU	A	28	32.202	10.758	23.013	1.00	31.67	C
C	LEU	A	28	33.223	11.167	24.054	1.00	32.22	C
O	LEU	A	28	33.013	10.970	25.258	1.00	33.37	O
CB	LEU	A	28	32.424	9.314	22.544	1.00	30.95	C
CG	LEU	A	28	31.228	8.660	21.830	1.00	30.19	C
CD1	LEU	A	28	31.560	7.271	21.337	1.00	28.60	C
CD2	LEU	A	28	30.002	8.622	22.744	1.00	29.86	C
N	ALA	A	29	34.295	11.843	23.649	1.00	32.19	N
CA	ALA	A	29	35.302	12.346	24.565	1.00	31.97	C
C	ALA	A	29	34.965	13.745	25.063	1.00	32.74	C
O	ALA	A	29	35.830	14.417	25.632	1.00	33.76	O
CB	ALA	A	29	36.675	12.342	23.893	1.00	30.85	C
N	GLY	A	30	33.761	14.238	24.824	1.00	32.92	N
CA	GLY	A	30	33.297	15.529	25.232	1.00	33.16	C
C	GLY	A	30	34.121	16.708	24.757	1.00	34.03	C
O	GLY	A	30	34.194	17.728	25.454	1.00	33.69	O
N	GLN	A	31	34.712	16.630	23.571	1.00	35.19	N
CA	GLN	A	31	35.478	17.738	23.014	1.00	36.06	C
C	GLN	A	31	34.564	18.823	22.454	1.00	35.59	C
O	GLN	A	31	33.447	18.518	22.014	1.00	36.40	O
CB	GLN	A	31	36.414	17.217	21.915	1.00	37.41	C
CG	GLN	A	31	37.802	16.866	22.389	1.00	39.45	C
CD	GLN	A	31	38.613	16.003	21.451	1.00	40.61	C
OE1	GLN	A	31	38.690	16.219	20.241	1.00	41.07	O
NE2	GLN	A	31	39.278	14.977	21.999	1.00	41.32	N
N	SER	A	32	35.018	20.075	22.452	1.00	33.36	N
CA	SER	A	32	34.222	21.154	21.881	1.00	32.18	C
C	SER	A	32	34.851	21.584	20.549	1.00	32.02	C
O	SER	A	32	36.060	21.425	20.377	1.00	32.16	O
CB	SER	A	32	34.092	22.344	22.816	1.00	31.37	C
OG	SER	A	32	33.391	23.419	22.212	1.00	29.60	O
N	GLY	A	33	34.043	22.121	19.642	1.00	30.46	N
CA	GLY	A	33	34.570	22.558	18.354	1.00	29.56	C
C	GLY	A	33	34.467	24.072	18.211	1.00	28.85	C
O	GLY	A	33	34.791	24.628	17.163	1.00	28.54	O
N	ILE	A	34	33.969	24.719	19.253	1.00	28.51	N
CA	ILE	A	34	33.770	26.156	19.246	1.00	29.03	C
C	ILE	A	34	35.088	26.919	19.316	1.00	31.01	C
O	ILE	A	34	36.044	26.565	20.003	1.00	31.09	O
CB	ILE	A	34	32.828	26.605	20.374	1.00	27.97	C
CG1	ILE	A	34	31.627					

2

CD2	LEU	A	36	36.741	34.337	20.280	1.00	33.48	C
N	ILE	A	37	36.144	33.366	15.713	1.00	32.62	N
CA	ILE	A	37	36.052	33.596	14.266	1.00	32.27	C
C	ILE	A	37	37.234	34.456	13.866	1.00	33.50	C
O	ILE	A	37	37.536	35.417	14.575	1.00	34.14	O
CB	ILE	A	37	34.730	34.316	13.961	1.00	31.61	C
CG1	ILE	A	37	33.573	33.312	13.932	1.00	30.43	C
CG2	ILE	A	37	34.812	35.106	12.666	1.00	31.81	C
CD1	ILE	A	37	32.227	33.902	14.284	1.00	29.18	C
N	ASP	A	38	37.947	34.146	12.798	1.00	36.45	N
CA	ASP	A	38	39.076	35.005	12.421	1.00	38.42	C
C	ASP	A	38	39.047	35.372	10.951	1.00	38.45	C
O	ASP	A	38	39.881	36.176	10.520	1.00	38.84	O
CB	ASP	A	38	40.394	34.326	12.797	1.00	40.40	C
CG	ASP	A	38	40.402	32.903	12.257	1.00	42.60	C
OD1	ASP	A	38	40.644	32.740	11.043	1.00	43.69	O
OD2	ASP	A	38	40.106	31.982	13.045	1.00	44.53	O
N	HIS	A	39	38.003	34.975	10.218	1.00	38.59	N
CA	HIS	A	39	37.926	35.284	8.792	1.00	38.54	C
C	HIS	A	39	37.217	36.591	8.487	1.00	38.34	C
O	HIS	A	39	37.094	36.980	7.321	1.00	38.38	O
CB	HIS	A	39	37.332	34.130	7.991	1.00	38.62	C
CG	HIS	A	39	36.023	33.615	8.480	1.00	39.30	C
ND1	HIS	A	39	35.901	32.834	9.610	1.00	40.20	N
CD2	HIS	A	39	34.768	33.780	7.997	1.00	39.04	C
CE1	HIS	A	39	34.625	32.533	9.798	1.00	39.85	C
NE2	HIS	A	39	33.921	33.101	8.833	1.00	39.44	N
N	PHE	A	40	36.775	37.315	9.496	1.00	38.47	N
CA	PHE	A	40	36.168	38.633	9.305	1.00	38.57	C
C	PHE	A	40	36.307	39.420	10.609	1.00	39.55	C
O	PHE	A	40	36.427	38.804	11.671	1.00	39.71	O
CB	PHE	A	40	34.758	38.544	8.806	1.00	37.77	C
CG	PHE	A	40	33.645	38.078	9.681	1.00	36.91	C
CD1	PHE	A	40	33.136	36.796	9.553	1.00	36.30	C
CD2	PHE	A	40	33.023	38.931	10.582	1.00	36.50	C
CE1	PHE	A	40	32.078	36.365	10.325	1.00	36.32	C
CE2	PHE	A	40	31.968	38.506	11.357	1.00	36.47	C
CZ	PHE	A	40	31.493	37.215	11.240	1.00	36.21	C
N	ASP	A	41	36.441	40.735	10.523	1.00	40.59	N
CA	ASP	A	41	36.619	41.528	11.749	1.00	42.02	C
C	ASP	A	41	35.370	41.430	12.610	1.00	41.11	C
O	ASP	A	41	34.291	41.785	12.136	1.00	41.74	O
CB	ASP	A	41	36.952	42.972	11.390	1.00	43.80	C
CG	ASP	A	41	37.737	43.667	12.486	1.00	45.45	C
OD1	ASP	A	41	38.750	43.090	12.935	1.00	46.51	O
OD2	ASP	A	41	37.345	44.779	12.895	1.00	46.80	O
N	THR	A	42	35.478	40.951	13.839	1.00	40.44	N
CA	THR	A	42	34.321	40.785	14.706			

Figure 2-5

CB	ALA	A	44	31.208	46.211	15.064	1.00	39.04	C
N	TYR	A	45	30.911	43.070	16.572	1.00	36.80	N
CA	TYR	A	45	29.924	42.025	16.761	1.00	35.25	C
C	TYR	A	45	29.768	41.583	18.197	1.00	34.29	C
O	TYR	A	45	30.735	41.526	18.958	1.00	35.60	O
CB	TYR	A	45	30.276	40.829	15.864	1.00	35.92	C
CG	TYR	A	45	30.039	41.091	14.391	1.00	36.02	C
CD1	TYR	A	45	30.930	41.877	13.664	1.00	36.12	C
CD2	TYR	A	45	28.944	40.551	13.727	1.00	35.78	C
CE1	TYR	A	45	30.721	42.140	12.321	1.00	35.54	C
CE2	TYR	A	45	28.735	40.799	12.380	1.00	35.49	C
CZ	TYR	A	45	29.621	41.592	11.692	1.00	35.82	C
OH	TYR	A	45	29.435	41.833	10.351	1.00	37.58	O
N	ALA	A	46	28.556	41.188	18.571	1.00	32.36	N
CA	ALA	A	46	28.245	40.750	19.929	1.00	31.00	C
C	ALA	A	46	28.587	39.287	20.162	1.00	30.09	C
O	ALA	A	46	28.536	38.763	21.281	1.00	30.77	O
CB	ALA	A	46	26.769	41.000	20.237	1.00	29.78	C
N	THR	A	47	28.832	38.560	19.098	1.00	29.39	N
CA	THR	A	47	29.274	37.171	19.162	1.00	29.14	C
C	THR	A	47	30.518	37.099	18.273	1.00	29.84	C
O	THR	A	47	30.500	37.554	17.120	1.00	29.99	O
CB	THR	A	47	28.209	36.160	18.763	1.00	28.64	C
OG1	THR	A	47	27.018	36.347	19.549	1.00	26.79	O
CG2	THR	A	47	28.730	34.739	18.992	1.00	27.92	C
N	LYS	A	48	31.607	36.614	18.844	1.00	30.40	N
CA	LYS	A	48	32.866	36.561	18.111	1.00	31.75	C
C	LYS	A	48	33.337	35.135	17.911	1.00	31.94	C
O	LYS	A	48	34.499	34.911	17.538	1.00	33.23	O
CB	LYS	A	48	33.936	37.388	18.833	1.00	33.40	C
CG	LYS	A	48	33.425	38.325	19.913	1.00	34.99	C
CD	LYS	A	48	34.435	39.384	20.296	1.00	36.14	C
CE	LYS	A	48	34.249	40.674	19.509	1.00	36.82	C
NZ	LYS	A	48	33.140	41.508	20.060	1.00	37.15	N
N	PHE	A	49	32.433	34.182	18.140	1.00	31.02	N
CA	PHE	A	49	32.807	32.777	18.010	1.00	30.48	C
C	PHE	A	49	31.747	31.913	17.344	1.00	30.81	C
O	PHE	A	49	30.561	32.225	17.292	1.00	30.88	O
CB	PHE	A	49	33.110	32.226	19.413	1.00	29.09	C
CG	PHE	A	49	31.914	32.281	20.325	1.00	28.73	C
CD1	PHE	A	49	31.032	31.225	20.409	1.00	28.37	C
CD2	PHE	A	49	31.685	33.400	21.114	1.00	28.99	C
CE1	PHE	A	49	29.947	31.281	21.267	1.00	29.19	C
CE2	PHE	A	49	30.593	33.466	21.957	1.00	28.39	C
CZ	PHE	A	49	29.720	32.401	22.041	1.00	28.17	C
N	ALA	A	50	32.193	30.761	16.845	1.00	31.01	N
CA	ALA	A	50	31.329	29.803	16.187	1.00	30.91	C
C	ALA	A	50	31.951	28.410	16.154	1.00	31.13	C

Figure 2-6

CA	VAL	A	53	35.180	23.418	10.060	1.00	36.67	C
C	VAL	A	53	36.657	23.748	9.883	1.00	39.49	C
O	VAL	A	53	36.983	24.713	9.185	1.00	39.50	O
CB	VAL	A	53	34.492	22.991	8.765	1.00	35.64	C
CG1	VAL	A	53	35.288	21.993	7.943	1.00	34.33	C
CG2	VAL	A	53	33.113	22.403	9.098	1.00	34.62	C
N	LYS	A	54	37.535	23.040	10.588	1.00	42.77	N
CA	LYS	A	54	38.955	23.337	10.595	1.00	46.02	C
C	LYS	A	54	39.807	22.528	9.634	1.00	48.60	C
O	LYS	A	54	39.695	21.320	9.468	1.00	48.51	O
CB	LYS	A	54	39.498	23.184	12.031	1.00	46.00	C
CG	LYS	A	54	38.765	24.095	13.013	1.00	46.36	C
CD	LYS	A	54	38.735	23.509	14.408	1.00	46.28	C
CE	LYS	A	54	37.330	23.395	14.954	1.00	46.49	C
NZ	LYS	A	54	36.792	24.669	15.488	1.00	46.54	N
N	ASP	A	55	40.730	23.244	8.991	1.00	52.11	N
CA	ASP	A	55	41.654	22.694	8.012	1.00	55.06	C
C	ASP	A	55	40.927	21.790	7.030	1.00	56.01	C
O	ASP	A	55	41.110	20.579	6.985	1.00	56.42	O
CB	ASP	A	55	42.813	21.976	8.707	1.00	56.66	C
CG	ASP	A	55	43.718	22.953	9.441	1.00	58.45	C
OD1	ASP	A	55	44.364	23.795	8.777	1.00	59.28	O
OD2	ASP	A	55	43.773	22.897	10.692	1.00	59.47	O
N	PHE	A	56	40.060	22.409	6.230	1.00	57.29	N
CA	PHE	A	56	39.245	21.657	5.276	1.00	58.33	C
C	PHE	A	56	39.919	21.613	3.915	1.00	59.60	C
O	PHE	A	56	40.252	22.646	3.339	1.00	60.07	O
CB	PHE	A	56	37.845	22.257	5.201	1.00	57.68	C
CG	PHE	A	56	37.061	21.988	3.953	1.00	56.82	C
CD1	PHE	A	56	36.509	20.746	3.707	1.00	56.49	C
CD2	PHE	A	56	36.868	22.997	3.019	1.00	56.58	C
CE1	PHE	A	56	35.791	20.514	2.548	1.00	56.82	C
CE2	PHE	A	56	36.143	22.774	1.868	1.00	56.36	C
CZ	PHE	A	56	35.602	21.526	1.630	1.00	56.45	C
N	ASN	A	57	40.137	20.409	3.416	1.00	61.48	N
CA	ASN	A	57	40.716	20.206	2.094	1.00	63.34	C
C	ASN	A	57	39.632	19.660	1.162	1.00	64.04	C
O	ASN	A	57	38.720	18.963	1.625	1.00	64.29	O
CB	ASN	A	57	41.890	19.230	2.145	1.00	64.21	C
CG	ASN	A	57	43.104	19.746	1.398	1.00	65.21	C
OD1	ASN	A	57	43.551	20.872	1.641	1.00	65.56	O
ND2	ASN	A	57	43.643	18.932	0.497	1.00	65.37	N
N	CYS	A	58	39.697	20.028	-0.111	1.00	64.22	N
CA	CYS	A	58	38.699	19.538	-1.061	1.00	64.43	C
C	CYS	A	58	39.324	19.389	-2.440	1.00	64.92	C
O	CYS	A	58	38.766	18.709	-3.292	1.00	64.47	O
CB	CYS	A	58	37.460	20.414	-1.089	1.00	64.20	C
SG	CYS	A	58	37.608	22.077	-1.749	1.00	63.44	S
N	GLU	A	59	40.546	19.874	-2			

Figure 2-7

OD1	ASP	A	60	42.745	16.618	-1.651	1.00	69.37	O
OD2	ASP	A	60	41.707	14.871	-0.819	1.00	69.27	O
N	ILE	A	61	39.022	16.292	-4.357	1.00	67.60	N
CA	ILE	A	61	37.674	16.071	-4.832	1.00	67.38	C
C	ILE	A	61	37.180	17.149	-5.787	1.00	67.54	C
O	ILE	A	61	36.497	16.848	-6.770	1.00	67.93	O
CB	ILE	A	61	36.667	15.988	-3.664	1.00	67.40	C
CG1	ILE	A	61	37.311	15.408	-2.413	1.00	67.80	C
CG2	ILE	A	61	35.449	15.180	-4.083	1.00	67.34	C
CD1	ILE	A	61	37.777	13.973	-2.513	1.00	68.03	C
N	ILE	A	62	37.391	18.412	-5.440	1.00	67.52	N
CA	ILE	A	62	36.982	19.529	-6.274	1.00	67.98	C
C	ILE	A	62	38.205	20.343	-6.706	1.00	68.48	C
O	ILE	A	62	38.999	20.776	-5.872	1.00	68.15	O
CB	ILE	A	62	35.993	20.477	-5.575	1.00	68.14	C
CG1	ILE	A	62	34.855	19.723	-4.881	1.00	67.67	C
CG2	ILE	A	62	35.412	21.476	-6.575	1.00	67.87	C
CD1	ILE	A	62	34.527	20.263	-3.510	1.00	67.28	C
N	SER	A	63	38.310	20.600	-8.002	1.00	69.51	N
CA	SER	A	63	39.417	21.370	-8.554	1.00	70.54	C
C	SER	A	63	39.290	22.856	-8.265	1.00	70.89	C
O	SER	A	63	38.176	23.377	-8.181	1.00	71.31	O
CB	SER	A	63	39.443	21.182	-10.081	1.00	71.01	C
OG	SER	A	63	38.191	21.601	-10.622	1.00	71.28	O
N	ARG	A	64	40.407	23.574	-8.237	1.00	71.13	N
CA	ARG	A	64	40.418	25.011	-7.990	1.00	70.88	C
C	ARG	A	64	39.638	25.800	-9.027	1.00	69.35	C
O	ARG	A	64	39.069	26.861	-8.737	1.00	69.23	O
CB	ARG	A	64	41.859	25.524	-7.905	1.00	72.62	C
CG	ARG	A	64	42.772	24.624	-7.080	1.00	74.72	C
CD	ARG	A	64	43.816	23.964	-7.969	1.00	76.13	C
NE	ARG	A	64	44.540	22.911	-7.262	1.00	77.32	N
CZ	ARG	A	64	45.834	22.661	-7.436	1.00	78.17	C
NH1	ARG	A	64	46.546	23.383	-8.294	1.00	78.63	N
NH2	ARG	A	64	46.395	21.679	-6.743	1.00	78.58	N
N	LYS	A	65	39.566	25.310	-10.259	1.00	67.53	N
CA	LYS	A	65	38.788	25.972	-11.298	1.00	65.69	C
C	LYS	A	65	37.295	25.760	-11.038	1.00	63.81	C
O	LYS	A	65	36.479	26.601	-11.405	1.00	63.43	O
CB	LYS	A	65	39.167	25.454	-12.682	1.00	66.44	C
CG	LYS	A	65	40.622	25.665	-13.056	1.00	67.23	C
CD	LYS	A	65	40.858	27.006	-13.722	1.00	67.48	C
CE	LYS	A	65	41.632	26.857	-15.022	1.00	67.88	C
NZ	LYS	A	65	41.367	27.998	-15.950	1.00	67.80	N
N	GLU	A	66	36.945	24.645	-10.402	1.00	61.40	N
CA	GLU	A	66	35.560	24.328	-10.097	1.00	59.42	C
C	GLU	A	66	35.121	24.864	-8.741	1.00	57.68	C
O	GLU	A	66	33.927	25.012	-8.469	1.00	57.07	O
CB	GLU	A	66	35.341	22.812	-10.174	1.00	59.70	C
CG	GLU	A	66	35.295	22.297	-11.605	1.00	60.10	C
CD	GLU	A	66	33.929	22.447	-12.245	1.00	60.14	C
OE1	GLU	A	66	33.820	23.096	-13.304	1.00	59.46	O
OE2	GLU	A	66	32.952	21.907	-11.682	1.00	60.54	O
N	GLN	A	67	36.076	25.201	-7.893	1.00	55.83	N
CA	GLN	A	67	35.842	25.754	-6.574	1.00	54.78	C
C	GLN	A	67	35.173	27.125	-6.634	1.00	53.83	C
O	GLN	A	67	34.343	27.470	-5.803	1.00	53.09	O
CB	GLN	A	67	37.175	25.908	-5.842	1.00	55.38	C
CG	GLN	A	67	37.455	24.916	-4.738	1.00	56.07	C
CD	GLN	A	67	38.776	25.233	-4.052	1.00	56.50	C
OE1	GLN	A	67	38.931	26.290	-3.447	1.00	56.45	O
NE2	GLN	A	67	39.720	24.308	-4.163	1.00	57.61	N
N	ARG	A	68	35.525	27.914	-7.632	1.00	53.40	N

Figure 2-8

CA	ARG	A	68	35.065	29.247	-7.896	1.00	52.43	C
C	ARG	A	68	33.615	29.368	-8.330	1.00	49.54	C
O	ARG	A	68	33.100	30.491	-8.400	1.00	49.30	O
CB	ARG	A	68	35.932	29.890	-9.011	1.00	55.50	C
CG	ARG	A	68	36.265	31.348	-8.741	1.00	58.96	C
CD	ARG	A	68	36.100	32.210	-9.982	1.00	61.92	C
NE	ARG	A	68	35.231	33.368	-9.770	1.00	64.11	N
CZ	ARG	A	68	35.580	34.490	-9.149	1.00	64.77	C
NH1	ARG	A	68	36.802	34.633	-8.651	1.00	65.05	N
NH2	ARG	A	68	34.710	35.487	-9.015	1.00	65.20	N
N	LYS	A	69	32.948	28.275	-8.649	1.00	45.91	N
CA	LYS	A	69	31.545	28.298	-9.044	1.00	43.05	C
C	LYS	A	69	30.648	27.848	-7.896	1.00	40.79	C
O	LYS	A	69	29.514	27.405	-8.079	1.00	40.97	O
CB	LYS	A	69	31.343	27.323	-10.216	1.00	42.96	C
CG	LYS	A	69	32.404	27.462	-11.299	1.00	43.11	C
CD	LYS	A	69	32.480	26.204	-12.151	1.00	42.58	C
CE	LYS	A	69	31.895	26.456	-13.532	1.00	42.02	C
NZ	LYS	A	69	32.812	25.970	-14.605	1.00	41.64	N
N	MET	A	70	31.191	27.869	-6.687	1.00	37.50	N
CA	MET	A	70	30.633	27.175	-5.555	1.00	34.98	C
C	MET	A	70	30.758	27.902	-4.223	1.00	32.38	C
O	MET	A	70	31.871	28.210	-3.798	1.00	32.03	O
CB	MET	A	70	31.425	25.864	-5.366	1.00	35.08	C
CG	MET	A	70	30.888	24.645	-6.066	1.00	35.01	C
SD	MET	A	70	31.957	23.217	-5.694	1.00	35.60	S
CE	MET	A	70	31.632	22.233	-7.165	1.00	35.07	C
N	ASP	A	71	29.633	28.071	-3.536	1.00	29.01	N
CA	ASP	A	71	29.750	28.647	-2.186	1.00	27.17	C
C	ASP	A	71	30.244	27.526	-1.274	1.00	26.77	C
O	ASP	A	71	30.018	26.329	-1.542	1.00	26.15	O
CB	ASP	A	71	28.432	29.242	-1.766	1.00	26.38	C
CG	ASP	A	71	28.364	29.693	-0.330	1.00	26.16	C
OD1	ASP	A	71	28.165	28.817	0.549	1.00	26.10	O
OD2	ASP	A	71	28.481	30.909	-0.081	1.00	25.93	O
N	ALA	A	72	30.909	27.882	-0.180	1.00	25.21	N
CA	ALA	A	72	31.419	26.919	0.780	1.00	23.86	C
C	ALA	A	72	30.381	25.913	1.237	1.00	23.27	C
O	ALA	A	72	30.727	24.742	1.469	1.00	23.23	O
CB	ALA	A	72	32.018	27.654	1.980	1.00	24.17	C
N	PHE	A	73	29.111	26.282	1.386	1.00	22.52	N
CA	PHE	A	73	28.109	25.289	1.788	1.00	22.41	C
C	PHE	A	73	28.012	24.159	0.777	1.00	23.21	C
O	PHE	A	73	27.924	22.992	1.186	1.00	24.39	O
CB	PHE	A	73	26.774	25.940	2.069	1.00	21.58	C
CG	PHE	A	73	25.743	25.898	0.995	1.00	20.70	C
CD1	PHE	A	73	24.736	24.944	1.023	1.00	20.86	C
CD2	PHE	A	73	25.785	26.798	-0.053	1.00	20.41	C
CE1	PHE	A	73	23.781	24.891	0.026			

Figure 2-9

CB	GLN	A	75	32.871	23.546	-0.806	1.00	26.42	C
CG	GLN	A	75	33.332	24.282	-2.062	1.00	28.06	C
CD	GLN	A	75	34.302	25.389	-1.689	1.00	29.61	C
OE1	GLN	A	75	35.078	25.201	-0.737	1.00	31.73	O
NE2	GLN	A	75	34.262	26.508	-2.390	1.00	28.55	N
N	TYR	A	76	31.183	21.843	1.155	1.00	25.75	N
CA	TYR	A	76	31.012	20.945	2.284	1.00	24.59	C
C	TYR	A	76	30.091	19.783	1.905	1.00	25.40	C
O	TYR	A	76	30.453	18.620	2.090	1.00	26.52	O
CB	TYR	A	76	30.418	21.710	3.456	1.00	23.32	C
CG	TYR	A	76	31.291	22.727	4.146	1.00	23.16	C
CD1	TYR	A	76	30.789	23.430	5.249	1.00	22.41	C
CD2	TYR	A	76	32.593	23.002	3.755	1.00	22.62	C
CE1	TYR	A	76	31.549	24.362	5.915	1.00	22.33	C
CE2	TYR	A	76	33.366	23.944	4.395	1.00	21.92	C
CZ	TYR	A	76	32.842	24.622	5.477	1.00	23.20	C
OH	TYR	A	76	33.608	25.548	6.155	1.00	22.62	O
N	GLY	A	77	28.927	20.091	1.335	1.00	24.29	N
CA	GLY	A	77	27.960	19.090	0.948	1.00	23.68	C
C	GLY	A	77	28.532	18.017	0.040	1.00	24.17	C
O	GLY	A	77	28.286	16.831	0.258	1.00	24.09	O
N	ILE	A	78	29.208	18.420	-1.031	1.00	24.69	N
CA	ILE	A	78	29.852	17.512	-1.963	1.00	24.28	C
C	ILE	A	78	30.854	16.603	-1.263	1.00	24.34	C
O	ILE	A	78	30.693	15.382	-1.276	1.00	24.29	O
CB	ILE	A	78	30.586	18.300	-3.074	1.00	24.14	C
CG1	ILE	A	78	29.568	19.116	-3.859	1.00	24.40	C
CG2	ILE	A	78	31.358	17.347	-3.975	1.00	24.03	C
CD1	ILE	A	78	30.086	19.834	-5.084	1.00	24.19	C
N	VAL	A	79	31.854	17.194	-0.603	1.00	23.70	N
CA	VAL	A	79	32.878	16.422	0.095	1.00	23.40	C
C	VAL	A	79	32.243	15.394	1.017	1.00	24.44	C
O	VAL	A	79	32.638	14.232	0.981	1.00	25.15	O
CB	VAL	A	79	33.858	17.307	0.874	1.00	23.00	C
CG1	VAL	A	79	34.656	16.524	1.907	1.00	22.25	C
CG2	VAL	A	79	34.830	18.006	-0.077	1.00	22.73	C
N	ALA	A	80	31.258	15.787	1.820	1.00	25.12	N
CA	ALA	A	80	30.575	14.849	2.700	1.00	25.90	C
C	ALA	A	80	29.765	13.840	1.895	1.00	27.36	C
O	ALA	A	80	29.609	12.695	2.314	1.00	28.42	O
CB	ALA	A	80	29.689	15.571	3.690	1.00	24.87	C
N	GLY	A	81	29.235	14.245	0.749	1.00	28.62	N
CA	GLY	A	81	28.466	13.337	-0.097	1.00	30.56	C
C	GLY	A	81	29.379	12.247	-0.652	1.00	32.31	C
O	GLY	A	81	29.048	11.061	-0.608	1.00	32.11	O
N	VAL	A	82	30.556	12.667	-1.132	1.00	32.99	N
CA	VAL	A	82	31.535	11.714	-1.646	1.00	33.88	C
C	VAL	A	82	31.827	10.661	-0.586	1.00	35.83	C
O	VAL	A	82	31.598	9.465	-0.785	1.00	37.36	O
CB	VAL	A	82	32.826	12.415	-2.082	1.00	33.65	C
CG1	VAL	A	82	33.943	11.418	-2.341	1.00	32.35	C
CG2	VAL	A	82	32.578	13.263	-3.334	1.00	33.37	C
N	GLN	A	83	32.170	11.110	0.617	1.00	36.36	N
CA	GLN	A	83	32.387	10.238	1.757	1.00	36.77	C
C	GLN	A	83	31.271	9.199	1.851	1.00	36.63	C
O	GLN	A	83	31.534	8.003	1.903	1.00	37.55	O
CB	GLN	A	83	32.437	11.041	3.056	1.00	36.97	C
CG	GLN	A	83	33.765	11.611	3.489	1.00	36.84	C
CD	GLN	A	83	33.698	12.194	4.888	1.00	38.07	C
OE1	GLN	A	83	33.123	11.581	5.796	1.00	39.74	O
NE2	GLN	A	83	34.247	13.375	5.119	1.00	37.60	N
N	ALA	A	84	30.028	9.661	1.864	1.00	36.63	N
CA	ALA	A	84	28.872	8.782	1.983	1.00	36.65	C

Figure 2-10

C	ALA	A	84	28.805	7.776	0.849	1.00	36.36	C
O	ALA	A	84	28.499	6.613	1.097	1.00	35.48	O
CB	ALA	A	84	27.592	9.595	2.089	1.00	36.13	C
N	MET	A	85	29.116	8.196	-0.367	1.00	37.76	N
CA	MET	A	85	29.111	7.287	-1.508	1.00	39.69	C
C	MET	A	85	30.223	6.257	-1.367	1.00	41.00	C
O	MET	A	85	30.009	5.060	-1.568	1.00	41.42	O
CB	MET	A	85	29.264	8.053	-2.820	1.00	40.12	C
CG	MET	A	85	28.061	8.945	-3.132	1.00	40.96	C
SD	MET	A	85	26.538	8.001	-3.315	1.00	41.36	S
CE	MET	A	85	26.973	6.931	-4.683	1.00	40.65	C
N	GLN	A	86	31.410	6.738	-0.992	1.00	42.08	N
CA	GLN	A	86	32.553	5.840	-0.817	1.00	42.74	C
C	GLN	A	86	32.252	4.822	0.259	1.00	42.97	C
O	GLN	A	86	32.169	3.616	-0.027	1.00	43.31	O
CB	GLN	A	86	33.823	6.663	-0.577	1.00	43.27	C
CG	GLN	A	86	34.312	7.257	-1.888	1.00	44.50	C
CD	GLN	A	86	35.480	8.188	-1.859	1.00	45.31	C
OE1	GLN	A	86	35.978	8.671	-0.844	1.00	45.76	O
NE2	GLN	A	86	35.975	8.516	-3.067	1.00	45.96	N
N	ASP	A	87	31.763	5.277	1.408	1.00	43.03	N
CA	ASP	A	87	31.337	4.384	2.470	1.00	44.15	C
C	ASP	A	87	30.274	3.396	2.008	1.00	45.71	C
O	ASP	A	87	30.250	2.245	2.453	1.00	46.35	O
CB	ASP	A	87	30.802	5.186	3.661	1.00	43.42	C
CG	ASP	A	87	30.677	4.330	4.904	1.00	43.34	C
OD1	ASP	A	87	31.598	3.517	5.157	1.00	44.06	O
OD2	ASP	A	87	29.677	4.458	5.632	1.00	42.70	O
N	SER	A	88	29.370	3.825	1.135	1.00	47.04	N
CA	SER	A	88	28.293	2.977	0.654	1.00	48.12	C
C	SER	A	88	28.814	1.828	-0.197	1.00	49.19	C
O	SER	A	88	28.259	0.731	-0.169	1.00	48.51	O
CB	SER	A	88	27.281	3.803	-0.145	1.00	47.96	C
OG	SER	A	88	27.686	3.947	-1.492	1.00	47.71	O
N	GLY	A	89	29.809	2.112	-1.033	1.00	50.61	N
CA	GLY	A	89	30.381	1.147	-1.945	1.00	52.39	C
C	GLY	A	89	29.514	0.870	-3.164	1.00	54.05	C
O	GLY	A	89	29.776	-0.068	-3.925	1.00	54.48	O
N	LEU	A	90	28.453	1.639	-3.374	1.00	55.16	N
CA	LEU	A	90	27.568	1.451	-4.506	1.00	56.38	C
C	LEU	A	90	28.365	1.603	-5.807	1.00	57.19	C
O	LEU	A	90	29.179	2.512	-5.927	1.00	56.97	O
CB	LEU	A	90	26.450	2.479	-4.548	1.00	56.95	C
CG	LEU	A	90	25.064	2.193	-4.018	1.00	57.07	C
CD1	LEU	A	90	24.119	3.328	-4.430	1.00	56.91	C
CD2	LEU	A	90	24.503	0.865	-4.490	1.00	57.14	C
N	GLU	A	91	28.000	0.803	-6.797	1.00	58.89	N
CA	GLU	A	91	28.532	1.023	-8.143	1.00	60.44	C
C	GLU	A	91	27.379	1.498	-9			

Figure 2-11

Figure 2-12

CD1	ILE	A	100	22.465	4.568	-8.720	1.00	34.52	C
N	GLY	A	101	18.781	8.612	-6.457	1.00	34.35	N
CA	GLY	A	101	18.555	10.059	-6.465	1.00	33.77	C
C	GLY	A	101	19.240	10.769	-5.308	1.00	33.33	C
O	GLY	A	101	20.126	10.214	-4.654	1.00	33.58	O
N	ALA	A	102	18.803	11.995	-5.024	1.00	32.06	N
CA	ALA	A	102	19.383	12.798	-3.953	1.00	30.82	C
C	ALA	A	102	18.332	13.668	-3.284	1.00	29.70	C
O	ALA	A	102	17.363	14.086	-3.909	1.00	31.01	O
CB	ALA	A	102	20.516	13.678	-4.479	1.00	30.53	C
N	ALA	A	103	18.512	13.933	-1.999	1.00	28.03	N
CA	ALA	A	103	17.575	14.753	-1.230	1.00	25.22	C
C	ALA	A	103	18.363	15.540	-0.184	1.00	23.85	C
O	ALA	A	103	18.559	15.134	0.952	1.00	23.10	O
CB	ALA	A	103	16.497	13.910	-0.595	1.00	24.51	C
N	ILE	A	104	19.019	16.587	-0.671	1.00	23.05	N
CA	ILE	A	104	19.908	17.401	0.135	1.00	22.38	C
C	ILE	A	104	19.394	18.834	0.207	1.00	22.22	C
O	ILE	A	104	19.072	19.399	-0.839	1.00	22.93	O
CB	ILE	A	104	21.327	17.415	-0.478	1.00	21.90	C
CG1	ILE	A	104	21.877	15.989	-0.520	1.00	21.01	C
CG2	ILE	A	104	22.239	18.354	0.291	1.00	21.57	C
CD1	ILE	A	104	22.977	15.754	-1.509	1.00	19.64	C
N	GLY	A	105	19.352	19.406	1.402	1.00	21.16	N
CA	GLY	A	105	18.934	20.783	1.569	1.00	20.18	C
C	GLY	A	105	19.941	21.613	2.354	1.00	19.37	C
O	GLY	A	105	21.043	21.222	2.690	1.00	19.81	O
N	SER	A	106	19.528	22.815	2.693	1.00	19.13	N
CA	SER	A	106	20.275	23.799	3.448	1.00	18.03	C
C	SER	A	106	19.252	24.795	4.004	1.00	19.00	C
O	SER	A	106	18.175	24.921	3.419	1.00	19.81	O
CB	SER	A	106	21.271	24.488	2.526	1.00	17.16	C
OG	SER	A	106	22.092	25.439	3.156	1.00	15.90	O
N	GLY	A	107	19.547	25.475	5.095	1.00	19.19	N
CA	GLY	A	107	18.639	26.453	5.655	1.00	18.05	C
C	GLY	A	107	18.625	27.702	4.781	1.00	18.77	C
O	GLY	A	107	17.531	28.123	4.418	1.00	18.68	O
N	ILE	A	108	19.781	28.295	4.496	1.00	19.98	N
CA	ILE	A	108	19.854	29.517	3.697	1.00	21.92	C
C	ILE	A	108	20.795	29.409	2.502	1.00	22.33	C
O	ILE	A	108	20.837	30.295	1.645	1.00	22.50	O
CB	ILE	A	108	20.293	30.744	4.526	1.00	22.68	C
CG1	ILE	A	108	19.999	32.067	3.812	1.00	22.56	C
CG2	ILE	A	108	21.790	30.677	4.834	1.00	22.23	C
CD1	ILE	A	108	18.740	32.773	4.209	1.00	22.91	C
N	GLY	A	109	21.596	28.356	2.417	1.00	23.23	N
CA	GLY	A	109	22.490	28.191	1.282	1.00	22.77	C
C	GLY	A	109	23.618	29.206	1.299	1.00	23.95	C
O	GLY	A	109	24.325	29.369	2.302	1.00	24.99	O
N	GLY	A	110	23.968	29.728	0.119	1.00	22.53	N
CA	GLY	A	110	25.186	30.444	-0.086	1.00	21.57	C
C	GLY	A	110	25.295	31.872	0.353	1.00	21.34	C
O	GLY	A	110	25.779	32.717	-0.426	1.00	20.36	O
N	LEU	A	111	25.141	32.142	1.646	1.00	21.33	N
CA	LEU	A	111	25.285	33.486	2.183	1.00	21.06	C
C	LEU	A	111	26.612	34.144	1.839	1.00	19.97	C
O	LEU	A	111	26.655	35.343	1.573	1.00	19.87	O
CB	LEU	A	111	25.107	33.458	3.709	1.00	21.38	C
CG	LEU	A	111	23.849	34.136	4.252	1.00	21.04	C
CD1	LEU	A	111	23.966	34.302	5.758	1.00	21.27	C
CD2	LEU	A	111	23.605	35.470	3.584	1.00	20.64	C
N	GLY	A	112	27.706	33.399	1.864	1.00	19.90	N
CA	GLY	A	112	29.025	33.909	1.563	1.00	19.57	C

Figure 2-13

C	GLY	A	112	29.093	34.582	0.202	1.00	19.83	C
O	GLY	A	112	29.436	35.763	0.110	1.00	19.16	O
N	LEU	A	113	28.660	33.865	-0.835	1.00	20.37	N
CA	LEU	A	113	28.717	34.373	-2.195	1.00	21.45	C
C	LEU	A	113	27.667	35.432	-2.470	1.00	22.87	C
O	LEU	A	113	27.887	36.287	-3.349	1.00	24.10	O
CB	LEU	A	113	28.668	33.257	-3.233	1.00	21.15	C
CG	LEU	A	113	29.966	32.437	-3.379	1.00	21.11	C
CD1	LEU	A	113	29.850	31.447	-4.527	1.00	20.06	C
CD2	LEU	A	113	31.172	33.342	-3.549	1.00	20.34	C
N	ILE	A	114	26.567	35.437	-1.726	1.00	23.17	N
CA	ILE	A	114	25.566	36.481	-1.922	1.00	23.67	C
C	ILE	A	114	26.153	37.807	-1.442	1.00	24.59	C
O	ILE	A	114	26.093	38.806	-2.156	1.00	24.19	O
CB	ILE	A	114	24.246	36.209	-1.205	1.00	23.59	C
CG1	ILE	A	114	23.614	34.926	-1.749	1.00	23.20	C
CG2	ILE	A	114	23.293	37.390	-1.373	1.00	23.96	C
CD1	ILE	A	114	22.368	34.488	-1.014	1.00	22.82	C
N	GLU	A	115	26.791	37.773	-0.274	1.00	26.24	N
CA	GLU	A	115	27.382	38.995	0.283	1.00	28.37	C
C	GLU	A	115	28.485	39.536	-0.625	1.00	29.01	C
O	GLU	A	115	28.597	40.732	-0.855	1.00	28.40	O
CB	GLU	A	115	27.927	38.748	1.682	1.00	28.58	C
CG	GLU	A	115	26.918	38.301	2.723	1.00	29.16	C
CD	GLU	A	115	27.594	38.057	4.056	1.00	30.83	C
OE1	GLU	A	115	27.136	37.229	4.861	1.00	31.28	O
OE2	GLU	A	115	28.643	38.695	4.293	1.00	32.63	O
N	GLU	A	116	29.313	38.632	-1.139	1.00	30.70	N
CA	GLU	A	116	30.396	38.976	-2.041	1.00	31.25	C
C	GLU	A	116	29.865	39.618	-3.315	1.00	29.86	C
O	GLU	A	116	30.328	40.689	-3.701	1.00	29.96	O
CB	GLU	A	116	31.211	37.729	-2.396	1.00	33.77	C
CG	GLU	A	116	32.443	38.037	-3.238	1.00	37.37	C
CD	GLU	A	116	33.380	36.848	-3.326	1.00	39.87	C
OE1	GLU	A	116	33.652	36.249	-2.253	1.00	41.44	O
OE2	GLU	A	116	33.825	36.519	-4.447	1.00	40.97	O
N	ASN	A	117	28.893	38.962	-3.954	1.00	27.58	N
CA	ASN	A	117	28.342	39.520	-5.195	1.00	25.34	C
C	ASN	A	117	27.694	40.865	-4.966	1.00	25.27	C
O	ASN	A	117	28.025	41.830	-5.663	1.00	25.06	O
CB	ASN	A	117	27.401	38.518	-5.849	1.00	23.78	C
CG	ASN	A	117	28.223	37.458	-6.584	1.00	23.22	C
OD1	ASN	A	117	28.593	37.682	-7.736	1.00	23.18	O
ND2	ASN	A	117	28.516	36.354	-5.929	1.00	22.14	N
N	HIS	A	118	26.877	40.991	-3.922	1.00	25.45	N
CA	HIS	A	118	26.234	42.236	-3.569	1.00	25.44	C
C	HIS	A	118	27.235	43.361	-3.319	1.00	26.62	C
O	HIS	A	118	27.016	44.496	-3.749	1.00	26.46	O
CB	HIS	A	118	25.330	42.060	-2.335	1.00	24.14	C
CG	HIS	A	118	24.462	43.273	-2.164	1.00	23.03	C
ND1	HIS	A	118	24.589	44.116	-1.095	1.00	23.14	N
CD2	HIS	A	118	23.480	43.774	-2.955	1.00	22.09	C
CE1	HIS	A	118	23.700	45.101	-1.220	1.00	22.98	C
NE2	HIS	A	118	23.026	44.916	-2.342	1.00	22.18	N
N	THR	A	119	28.347	43.054	-2.668	1.00	27.91	N
CA	THR	A	119	29.438	43.991	-2.456	1.00	29.63	C
C	THR	A	119	29.983	44.489	-3.790	1.00	30.90	C
O	THR	A	119	29.968	45.696	-4.060	1.00	32.10	O
CB	THR	A	119	30.574	43.315	-1.665	1.00	29.98	C
OG1	THR	A	119	30.019	42.865	-0.421	1.00	30.86	O
CG2	THR	A	119	31.718	44.270	-1.392	1.00	29.85	C
N	SER	A	120	30.316	43.565	-4.687	1.00	31.36	N
CA	SER	A	120	30.777	43.912	-6.021	1.00	33.00	C

Figure 2-14

1198	O	CYS	A	163	16.667	21.756	11.814	1.00	21.45
1199	CB	CYS	A	163	16.880	24.441	12.673	1.00	24.71
1200	SG	CYS	A	163	17.913	25.911	12.915	1.00	28.93
1201	N	THR	A	164	15.037	22.488	10.446	1.00	21.76
1202	CA	THR	A	164	14.453	21.156	10.329	1.00	21.16
1203	C	THR	A	164	14.888	20.517	9.020	1.00	20.59
1204	O	THR	A	164	14.714	19.323	8.840	1.00	20.83
1205	CB	THR	A	164	12.927	21.172	10.433	1.00	20.78
1206	OG1	THR	A	164	12.549	22.030	11.519	1.00	21.06
1207	CG2	THR	A	164	12.396	19.772	10.675	1.00	20.38
1208	N	SER	A	165	15.513	21.302	8.153	1.00	21.25
1209	CA	SER	A	165	15.984	20.830	6.858	1.00	21.35
1210	C	SER	A	165	16.609	19.451	6.925	1.00	21.57
1211	O	SER	A	165	16.155	18.544	6.235	1.00	21.53
1212	CB	SER	A	165	17.007	21.809	6.265	1.00	20.98
1213	OG	SER	A	165	16.371	23.066	6.071	1.00	21.82
1214	N	GLY	A	166	17.618	19.286	7.774	1.00	22.48
1215	CA	GLY	A	166	18.315	18.020	7.925	1.00	22.79
1216	C	GLY	A	166	17.388	16.830	8.069	1.00	22.94
1217	O	GLY	A	166	17.567	15.809	7.409	1.00	22.55
1218	N	VAL	A	167	16.444	16.936	9.004	1.00	23.72
1219	CA	VAL	A	167	15.506	15.848	9.271	1.00	24.29
1220	C	VAL	A	167	14.558	15.638	8.109	1.00	24.54
1221	O	VAL	A	167	14.389	14.509	7.627	1.00	26.12
1222	CB	VAL	A	167	14.767	16.094	10.592	1.00	24.57
1223	CG1	VAL	A	167	13.442	15.358	10.672	1.00	25.23
1224	CG2	VAL	A	167	15.675	15.663	11.743	1.00	24.67
1225	N	HIS	A	168	13.991	16.711	7.572	1.00	24.23
1226	CA	HIS	A	168	13.060	16.594	6.455	1.00	23.72
1227	C	HIS	A	168	13.671	15.915	5.243	1.00	23.37
1228	O	HIS	A	168	13.003	15.055	4.637	1.00	24.37
1229	CB	HIS	A	168	12.494	17.964	6.099	1.00	23.34
1230	CG	HIS	A	168	11.429	18.457	7.027	1.00	23.31
1231	ND1	HIS	A	168	11.102	19.797	7.120	1.00	22.78
1232	CD2	HIS	A	168	10.613	17.813	7.897	1.00	22.79
1233	CE1	HIS	A	168	10.138	19.951	8.014	1.00	22.01
1234	NE2	HIS	A	168	9.823	18.768	8.491	1.00	21.89
1235	N	ASN	A	169	14.898	16.225	4.857	1.00	22.74
1236	CA	ASN	A	169	15.502	15.616	3.663	1.00	23.00
1237	C	ASN	A	169	15.656	14.107	3.822	1.00	23.66
1238	O	ASN	A	169	15.361	13.299	2.934	1.00	23.83
1239	CB	ASN	A	169	16.826	16.291	3.343	1.00	22.66
1240	CG	ASN	A	169	16.710	17.635	2.662	1.00	22.82
1241	OD1	ASN	A	169	16.286	17.729	1.503	1.00	23.41
1242	ND2	ASN	A	169	17.107	18.717	3.315	1.00	21.89
1243	N	ILE	A	170	16.075	13.671	5.005	1.00	23.82
1244	CA	ILE	A	170	16.178	12.241	5.309	1.00	23.18
1245	C	ILE	A	170	14.784	11.637	5.275	1.00	22.89
1246	O	ILE	A	170	14.532	10.695	4.507	1.00	22.87
1247	CB	ILE	A	170	16.917	12.046	6.638	1.00	23.01
1248	CG1	ILE	A	170	18.322	12.677	6.508	1.00	22.40
1249	CG2	ILE	A	170	17.081	10.591	7.028	1.00	23.08
1250	CD1	ILE	A	170	18.989	12.935	7.825	1.00	22.78
1251	N	GLY	A	171	13.831	12.245	5.971	1.00	21.80
1252	CA	GLY	A	171	12.455	11.775	5.969	1.00	22.22
1253	C	GLY	A	171	11.908	11.490	4.579	1.00	22.83
1254	O	GLY	A	171	11.509	10.362	4.256	1.00	22.22
1255	N	HIS	A	172	11.918	12.497	3.702	1.00	23.21
1256	CA	HIS	A	172	11.335	12.357	2.369	1.00	22.97
1257	C	HIS	A	172	12.167	11.493	1.464	1.00	23.20
1258	O	HIS	A	172	11.668	10.866	0.520	1.00	23.49
1259	CB	HIS	A	172	11.036	13.753	1.771	1.00	22.55
1260	CG	HIS	A	172	9.823	14.271	2.506	1.00	22.55

Figure 2-20

1261	ND1	HIS	A	172	9.944	15.054	3.631	1.00	23.32
1262	CD2	HIS	A	172	8.513	14.044	2.327	1.00	22.72
1263	CE1	HIS	A	172	8.734	15.323	4.101	1.00	23.47
1264	NE2	HIS	A	172	7.844	14.717	3.329	1.00	23.29
1265	N	ALA	A	173	13.468	11.384	1.760	1.00	23.72
1266	CA	ALA	A	173	14.295	10.496	0.929	1.00	23.93
1267	C	ALA	A	173	13.810	9.058	1.148	1.00	23.83
1268	O	ALA	A	173	13.592	8.348	0.172	1.00	22.86
1269	CB	ALA	A	173	15.756	10.702	1.222	1.00	23.75
1270	N	ALA	A	174	13.506	8.691	2.390	1.00	23.88
1271	CA	ALA	A	174	12.985	7.375	2.714	1.00	24.96
1272	C	ALA	A	174	11.596	7.165	2.100	1.00	26.35
1273	O	ALA	A	174	11.326	6.134	1.482	1.00	26.24
1274	CB	ALA	A	174	12.865	7.184	4.215	1.00	24.24
1275	N	ARG	A	175	10.748	8.179	2.291	1.00	26.16
1276	CA	ARG	A	175	9.394	8.145	1.742	1.00	25.10
1277	C	ARG	A	175	9.481	7.878	0.245	1.00	27.12
1278	O	ARG	A	175	9.021	6.838	-0.251	1.00	28.18
1279	CB	ARG	A	175	8.673	9.443	2.042	1.00	23.30
1280	CG	ARG	A	175	8.348	9.684	3.507	1.00	23.23
1281	CD	ARG	A	175	7.206	8.809	3.977	1.00	23.38
1282	NE	ARG	A	175	6.465	9.357	5.099	1.00	24.63
1283	CZ	ARG	A	175	6.601	8.994	6.376	1.00	24.68
1284	NH1	ARG	A	175	7.476	8.054	6.731	1.00	24.38
1285	NH2	ARG	A	175	5.855	9.564	7.315	1.00	23.89
1286	N	ILE	A	176	10.257	8.703	-0.472	1.00	27.46
1287	CA	ILE	A	176	10.475	8.452	-1.893	1.00	27.19
1288	C	ILE	A	176	10.815	6.991	-2.141	1.00	28.06
1289	O	ILE	A	176	10.169	6.352	-2.971	1.00	29.01
1290	CB	ILE	A	176	11.568	9.372	-2.460	1.00	26.47
1291	CG1	ILE	A	176	11.036	10.812	-2.486	1.00	26.78
1292	CG2	ILE	A	176	12.020	8.935	-3.838	1.00	24.93
1293	CD1	ILE	A	176	11.966	11.826	-3.111	1.00	26.82
1294	N	ILE	A	177	11.823	6.460	-1.463	1.00	28.98
1295	CA	ILE	A	177	12.249	5.076	-1.652	1.00	29.01
1296	C	ILE	A	177	11.104	4.111	-1.387	1.00	29.49
1297	O	ILE	A	177	10.698	3.373	-2.290	1.00	30.21
1298	CB	ILE	A	177	13.483	4.745	-0.802	1.00	28.06
1299	CG1	ILE	A	177	14.718	5.428	-1.400	1.00	27.28
1300	CG2	ILE	A	177	13.712	3.245	-0.714	1.00	28.49
1301	CD1	ILE	A	177	15.924	5.483	-0.490	1.00	26.54
1302	N	ALA	A	178	10.479	4.215	-0.232	1.00	29.79
1303	CA	ALA	A	178	9.318	3.437	0.141	1.00	30.54
1304	C	ALA	A	178	8.251	3.453	-0.942	1.00	33.08
1305	O	ALA	A	178	7.640	2.422	-1.259	1.00	35.55
1306	CB	ALA	A	178	8.744	3.986	1.448	1.00	28.37
1307	N	TYR	A	179	7.975	4.621	-1.514	1.00	33.83
1308	CA	TYR	A	179	6.967	4.771	-2.546	1.00	33.95
1309	C	TYR	A	179	7.321	3.984	-3.798	1.00	33.95
1310	O	TYR	A	179	6.399	3.530	-4.495	1.00	35.65
1311	CB	TYR	A	179	6.779	6.254	-2.886	1.00	34.35
1312	CG	TYR	A	179	5.600	6.559	-3.781	1.00	34.82
1313	CD1	TYR	A	179	4.368	6.895	-3.228	1.00	35.00
1314	CD2	TYR	A	179	5.715	6.518	-5.167	1.00	34.57
1315	CE1	TYR	A	179	3.283	7.174	-4.034	1.00	35.41
1316	CE2	TYR	A	179	4.636	6.794	-5.976	1.00	34.96
1317	CZ	TYR	A	179	3.423	7.119	-5.404	1.00	35.48
1318	OH	TYR	A	179	2.338	7.399	-6.205	1.00	36.21
1319	N	GLY	A	180	8.590	3.866	-4.149	1.00	33.30
1320	CA	GLY	A	180	8.991	3.165	-5.356	1.00	33.89
1321	C	GLY	A	180	9.629	4.044	-6.418	1.00	34.58
1322	O	GLY	A	180	10.091	3.541	-7.461	1.00	34.05
1323	N	ASP	A	181	9.796	5.342	-6.136	1.00	34.25

Figure 2-21

1324	CA	ASP	A	181	10.383	6.259	-7.105	1.00	34.14
1325	C	ASP	A	181	11.898	6.108	-7.189	1.00	34.08
1326	O	ASP	A	181	12.531	6.521	-8.164	1.00	32.76
1327	CB	ASP	A	181	10.023	7.712	-6.773	1.00	34.55
1328	CG	ASP	A	181	8.564	8.032	-7.022	1.00	35.35
1329	OD1	ASP	A	181	7.996	8.921	-6.347	1.00	35.15
1330	OD2	ASP	A	181	7.975	7.377	-7.915	1.00	36.69
1331	N	ALA	A	182	12.486	5.534	-6.145	1.00	34.99
1332	CA	ALA	A	182	13.926	5.339	-6.075	1.00	35.64
1333	C	ALA	A	182	14.284	4.134	-5.210	1.00	36.12
1334	O	ALA	A	182	13.482	3.675	-4.395	1.00	36.49
1335	CB	ALA	A	182	14.594	6.592	-5.527	1.00	34.86
1336	N	ASP	A	183	15.496	3.630	-5.413	1.00	37.16
1337	CA	ASP	A	183	15.993	2.489	-4.644	1.00	37.73
1338	C	ASP	A	183	17.068	2.946	-3.662	1.00	37.03
1339	O	ASP	A	183	17.237	2.401	-2.575	1.00	37.13
1340	CB	ASP	A	183	16.558	1.416	-5.579	1.00	38.47
1341	CG	ASP	A	183	15.452	0.660	-6.299	1.00	39.28
1342	OD1	ASP	A	183	15.650	0.298	-7.477	1.00	39.31
1343	OD2	ASP	A	183	14.382	0.452	-5.672	1.00	39.27
1344	N	VAL	A	184	17.870	3.907	-4.112	1.00	35.93
1345	CA	VAL	A	184	18.906	4.529	-3.313	1.00	34.94
1346	C	VAL	A	184	18.726	6.051	-3.354	1.00	34.49
1347	O	VAL	A	184	18.388	6.611	-4.397	1.00	34.37
1348	CB	VAL	A	184	20.329	4.191	-3.783	1.00	34.92
1349	CG1	VAL	A	184	21.361	4.899	-2.904	1.00	34.98
1350	CG2	VAL	A	184	20.598	2.699	-3.774	1.00	34.24
1351	N	MET	A	185	18.909	6.700	-2.208	1.00	33.85
1352	CA	MET	A	185	18.808	8.150	-2.102	1.00	32.05
1353	C	MET	A	185	19.974	8.691	-1.280	1.00	30.49
1354	O	MET	A	185	20.234	8.138	-0.210	1.00	31.31
1355	CB	MET	A	185	17.503	8.560	-1.421	1.00	32.72
1356	CG	MET	A	185	16.248	8.454	-2.273	1.00	32.82
1357	SD	MET	A	185	16.312	9.494	-3.751	1.00	32.53
1358	CE	MET	A	185	15.762	11.052	-3.035	1.00	33.06
1359	N	VAL	A	186	20.675	9.701	-1.759	1.00	29.07
1360	CA	VAL	A	186	21.696	10.370	-0.952	1.00	27.75
1361	C	VAL	A	186	20.996	11.510	-0.206	1.00	26.95
1362	O	VAL	A	186	20.426	12.381	-0.880	1.00	28.34
1363	CB	VAL	A	186	22.846	10.975	-1.755	1.00	27.97
1364	CG1	VAL	A	186	24.006	11.307	-0.815	1.00	27.63
1365	CG2	VAL	A	186	23.324	10.065	-2.869	1.00	28.61
1366	N	ALA	A	187	20.997	11.526	1.114	1.00	24.74
1367	CA	ALA	A	187	20.259	12.588	1.793	1.00	24.07
1368	C	ALA	A	187	21.001	13.252	2.926	1.00	24.02
1369	O	ALA	A	187	21.836	12.664	3.607	1.00	24.74
1370	CB	ALA	A	187	18.942	1			

Figure 2-22

1387	O	GLU	A	191	27.522	24.903	6.772	1.00	18.20
1388	CB	GLU	A	191	24.313	24.973	7.186	1.00	18.97
1389	CG	GLU	A	191	23.760	26.391	7.329	1.00	20.04
1390	CD	GLU	A	191	22.420	26.607	6.662	1.00	20.10
1391	OE1	GLU	A	191	22.312	27.479	5.775	1.00	20.35
1392	OE2	GLU	A	191	21.423	25.921	6.984	1.00	19.18
1393	N	LYS	A	192	26.650	26.784	5.942	1.00	18.47
1394	CA	LYS	A	192	27.831	27.586	6.205	1.00	18.91
1395	C	LYS	A	192	27.392	29.047	6.334	1.00	19.50
1396	O	LYS	A	192	27.558	29.853	5.424	1.00	18.72
1397	CB	LYS	A	192	28.882	27.398	5.129	1.00	20.21
1398	CG	LYS	A	192	30.311	27.620	5.611	1.00	21.28
1399	CD	LYS	A	192	30.626	29.114	5.727	1.00	20.99
1400	CE	LYS	A	192	32.101	29.304	6.035	1.00	21.43
1401	NZ	LYS	A	192	32.369	30.319	7.082	1.00	20.87
1402	N	ALA	A	193	26.769	29.332	7.486	1.00	19.33
1403	CA	ALA	A	193	26.218	30.651	7.745	1.00	18.76
1404	C	ALA	A	193	27.125	31.471	8.633	1.00	20.38
1405	O	ALA	A	193	26.765	32.618	8.971	1.00	22.59
1406	CB	ALA	A	193	24.820	30.556	8.351	1.00	16.60
1407	N	SER	A	194	28.319	31.002	8.993	1.00	20.01
1408	CA	SER	A	194	29.212	31.816	9.822	1.00	19.73
1409	C	SER	A	194	29.827	32.946	9.010	1.00	19.70
1410	O	SER	A	194	31.018	32.969	8.692	1.00	19.94
1411	CB	SER	A	194	30.324	30.953	10.417	1.00	20.42
1412	OG	SER	A	194	31.139	30.457	9.359	1.00	20.95
1413	N	THR	A	195	29.005	33.897	8.600	1.00	19.16
1414	CA	THR	A	195	29.367	35.036	7.795	1.00	19.39
1415	C	THR	A	195	28.812	36.284	8.470	1.00	19.65
1416	O	THR	A	195	27.838	36.181	9.227	1.00	21.37
1417	CB	THR	A	195	28.757	34.967	6.382	1.00	20.32
1418	OG1	THR	A	195	27.366	35.354	6.457	1.00	21.29
1419	CG2	THR	A	195	28.843	33.585	5.772	1.00	19.40
1420	N	PRO	A	196	29.327	37.442	8.125	1.00	19.54
1421	CA	PRO	A	196	28.846	38.693	8.699	1.00	19.97
1422	C	PRO	A	196	27.341	38.754	8.825	1.00	19.83
1423	O	PRO	A	196	26.816	38.911	9.924	1.00	20.28
1424	CB	PRO	A	196	29.417	39.747	7.753	1.00	19.47
1425	CG	PRO	A	196	30.666	39.142	7.224	1.00	17.90
1426	CD	PRO	A	196	30.447	37.658	7.185	1.00	18.39
1427	N	LEU	A	197	26.601	38.575	7.744	1.00	21.07
1428	CA	LEU	A	197	25.156	38.631	7.691	1.00	21.15
1429	C	LEU	A	197	24.471	37.549	8.504	1.00	22.25
1430	O	LEU	A	197	23.391	37.781	9.057	1.00	22.33
1431	CB	LEU	A	197	24.696	38.550	6.235	1.00	20.97
1432	CG	LEU	A	197	23.530	39.417	5.781	1.00	20.00
1433	CD1	LEU	A	197	23.781	40.878	6.083	1.00	19.91
1434	CD2	LEU	A	197	23.283	39.197	4.290	1.00	19.18
1435	N	GLY	A	198	25.069	36.366	8.579	1.00	22.88
1436	CA	GLY	A	198	24.470	35.281	9.356	1.00	23.85
1437	C	GLY	A	198	24.739	35.506	10.839	1.00	26.11
1438	O	GLY	A	198	23.874	35.251	11.681	1.00	26.78
1439	N	VAL	A	199	25.956	35.969	11.160	1.00	26.93
1440	CA	VAL	A	199	26.250	36.222	12.587	1.00	27.85
1441	C	VAL	A	199	25.514	37.487	13.008	1.00	27.33
1442	O	VAL	A	199	24.683	37.455	13.926	1.00	27.42
1443	CB	VAL	A	199	27.746	36.267	12.877	1.00	28.42
1444	CG1	VAL	A	199	28.068	36.897	14.220	1.00	27.28
1445	CG2	VAL	A	199	28.327	34.844	12.826	1.00	27.96
1446	N	GLY	A	200	25.717	38.569	12.268	1.00	25.86
1447	CA	GLY	A	200	24.993	39.806	12.549	1.00	25.88
1448	C	GLY	A	200	23.493	39.535	12.646	1.00	25.97
1449	O	GLY	A	200	22.870	39.851	13.652	1.00	26.80

Figure 2-23

1450	N	GLY	A	201	22.885	38.974	11.615	1.00	25.48
1451	CA	GLY	A	201	21.478	38.693	11.546	1.00	25.31
1452	C	GLY	A	201	20.889	37.981	12.738	1.00	25.85
1453	O	GLY	A	201	19.849	38.418	13.259	1.00	25.85
1454	N	PHE	A	202	21.504	36.891	13.204	1.00	25.57
1455	CA	PHE	A	202	20.975	36.198	14.378	1.00	26.27
1456	C	PHE	A	202	21.237	37.041	15.627	1.00	27.19
1457	O	PHE	A	202	20.509	36.959	16.608	1.00	28.35
1458	CB	PHE	A	202	21.580	34.811	14.551	1.00	26.19
1459	CG	PHE	A	202	20.943	33.711	13.752	1.00	25.12
1460	CD1	PHE	A	202	21.643	33.073	12.738	1.00	24.21
1461	CD2	PHE	A	202	19.632	33.332	13.996	1.00	24.42
1462	CE1	PHE	A	202	21.051	32.076	11.991	1.00	23.44
1463	CE2	PHE	A	202	19.038	32.320	13.267	1.00	24.39
1464	CZ	PHE	A	202	19.752	31.695	12.257	1.00	23.79
1465	N	GLY	A	203	22.305	37.834	15.611	1.00	28.07
1466	CA	GLY	A	203	22.617	38.752	16.703	1.00	28.36
1467	C	GLY	A	203	21.489	39.776	16.825	1.00	29.38
1468	O	GLY	A	203	20.966	40.052	17.911	1.00	30.32
1469	N	ALA	A	204	21.089	40.312	15.677	1.00	28.66
1470	CA	ALA	A	204	20.027	41.289	15.581	1.00	28.43
1471	C	ALA	A	204	18.768	40.815	16.294	1.00	28.66
1472	O	ALA	A	204	18.131	41.610	16.982	1.00	29.26
1473	CB	ALA	A	204	19.743	41.609	14.117	1.00	28.52
1474	N	ALA	A	205	18.435	39.539	16.198	1.00	29.22
1475	CA	ALA	A	205	17.292	38.917	16.821	1.00	29.54
1476	C	ALA	A	205	17.532	38.582	18.293	1.00	30.76
1477	O	ALA	A	205	16.604	38.153	18.987	1.00	31.16
1478	CB	ALA	A	205	16.930	37.619	16.106	1.00	28.27
1479	N	ARG	A	206	18.779	38.677	18.735	1.00	31.45
1480	CA	ARG	A	206	19.159	38.399	20.110	1.00	32.71
1481	C	ARG	A	206	19.060	36.919	20.439	1.00	32.08
1482	O	ARG	A	206	18.810	36.532	21.575	1.00	32.74
1483	CB	ARG	A	206	18.299	39.212	21.090	1.00	33.69
1484	CG	ARG	A	206	18.709	40.680	21.147	1.00	35.43
1485	CD	ARG	A	206	18.168	41.326	22.416	1.00	37.32
1486	NE	ARG	A	206	18.714	40.674	23.601	1.00	38.75
1487	CZ	ARG	A	206	18.015	40.193	24.619	1.00	39.28
1488	NH1	ARG	A	206	18.676	39.617	25.623	1.00	40.09
1489	NH2	ARG	A	206	16.692	40.273	24.653	1.00	39.00
1490	N	ALA	A	207	19.351	36.086	19.459	1.00	31.89
1491	CA	ALA	A	207	19.203	34.651	19.541	1.00	30.97
1492	C	ALA	A	207	20.506	33.926	19.828	1.00	29.87
1493	O	ALA	A	207	20.485	32.707	20.028	1.00	30.21
1494	CB	ALA	A	207	18.657	34.153	18.183	1.00	30.74
1495	N	LEU	A	208	21.630	34.631	19.784	1.00	28.48
1496	CA	LEU	A	208	22.909	33.963	19.961	1.00	29.11
1497	C	LEU	A	208	23.516	34.215	21.336	1.00	29.38
1498	O	LEU	A	208	23.357	35.310	21.857	1.00	29.54
1499	CB	LEU	A	208	23.948	34.424	18.927	1.00	28.64
1500	CG	LEU	A	208	23.703	33.986	17.481	1.00	28.52
1501	CD1	LEU	A	208	24.704	34.659	16.558	1.00	27.66
1502	CD2	LEU	A	208	23.763	32.470	17.372	1.00	28.39
1503	N	SER	A	209	24.285	33.229	21.813	1.00	28.67
1504	CA	SER	A	209	24.999	33.395	23.072	1.00	27.73
1505	C	SER	A	209	26.090	34.453	22.903	1.00	27.76
1506	O	SER	A	209	26.493	34.797	21.800	1.00	26.99
1507	CB	SER	A	209	25.577	32.082	23.574	1.00	27.07
1508	OG	SER	A	209	26.481	32.291	24.653	1.00	26.06
1509	N	THR	A	210	26.482	35.063	24.008	1.00	29.62
1510	CA	THR	A	210	27.378	36.244	23.938	1.00	31.15
1511	C	THR	A	210	28.562	36.040	24.849	1.00	31.71
1512	O	THR	A	210	29.417	36.890	25.097	1.00	30.55

Figure 2-24

1513	CB	THR	A	210	26.495	37.458	24.255	1.00	31.98
1514	OG1	THR	A	210	26.238	38.187	23.037	1.00	32.30
1515	CG2	THR	A	210	27.039	38.393	25.302	1.00	32.74
1516	N	ARG	A	211	28.724	34.788	25.303	1.00	32.86
1517	CA	ARG	A	211	29.800	34.414	26.204	1.00	34.98
1518	C	ARG	A	211	31.142	34.331	25.505	1.00	35.34
1519	O	ARG	A	211	31.736	33.260	25.391	1.00	35.29
1520	CB	ARG	A	211	29.440	33.084	26.873	1.00	36.96
1521	CG	ARG	A	211	30.276	32.715	28.078	1.00	38.63
1522	CD	ARG	A	211	29.809	31.412	28.695	1.00	40.89
1523	NE	ARG	A	211	28.812	31.617	29.748	1.00	43.18
1524	CZ	ARG	A	211	27.497	31.538	29.556	1.00	44.37
1525	NH1	ARG	A	211	27.003	31.259	28.347	1.00	44.55
1526	NH2	ARG	A	211	26.676	31.740	30.581	1.00	44.44
1527	N	ASN	A	212	31.697	35.456	25.076	1.00	36.69
1528	CA	ASN	A	212	32.967	35.519	24.386	1.00	38.57
1529	C	ASN	A	212	34.172	35.285	25.283	1.00	40.78
1530	O	ASN	A	212	35.272	35.059	24.758	1.00	41.25
1531	CB	ASN	A	212	33.125	36.873	23.686	1.00	38.25
1532	CG	ASN	A	212	31.919	37.286	22.873	1.00	38.78
1533	OD1	ASN	A	212	31.326	36.500	22.126	1.00	38.93
1534	ND2	ASN	A	212	31.525	38.552	23.005	1.00	38.26
1535	N	ASP	A	213	34.018	35.328	26.601	1.00	43.10
1536	CA	ASP	A	213	35.130	35.122	27.525	1.00	45.40
1537	C	ASP	A	213	35.433	33.638	27.704	1.00	45.34
1538	O	ASP	A	213	36.540	33.257	28.080	1.00	44.99
1539	CB	ASP	A	213	34.896	35.821	28.858	1.00	47.21
1540	CG	ASP	A	213	33.652	35.405	29.603	1.00	49.21
1541	OD1	ASP	A	213	32.526	35.562	29.072	1.00	50.18
1542	OD2	ASP	A	213	33.789	34.906	30.749	1.00	50.24
1543	N	ASN	A	214	34.465	32.787	27.385	1.00	45.48
1544	CA	ASN	A	214	34.649	31.342	27.426	1.00	45.22
1545	C	ASN	A	214	33.840	30.670	26.316	1.00	43.77
1546	O	ASN	A	214	32.803	30.045	26.541	1.00	43.50
1547	CB	ASN	A	214	34.289	30.771	28.789	1.00	46.06
1548	CG	ASN	A	214	34.875	29.392	29.028	1.00	46.69
1549	OD1	ASN	A	214	35.114	29.005	30.174	1.00	47.37
1550	ND2	ASN	A	214	35.114	28.633	27.966	1.00	46.96
1551	N	PRO	A	215	34.345	30.763	25.089	1.00	42.47
1552	CA	PRO	A	215	33.653	30.271	23.911	1.00	41.85
1553	C	PRO	A	215	33.196	28.836	23.992	1.00	40.97
1554	O	PRO	A	215	32.078	28.509	23.586	1.00	40.92
1555	CB	PRO	A	215	34.665	30.467	22.785	1.00	41.51
1556	CG	PRO	A	215	35.519	31.597	23.234	1.00	41.27
1557	CD	PRO	A	215	35.569	31.517	24.730	1.00	41.71
1558	N	GLN	A	216	34.006	27.940	24.542	1.00	40.36
1559	CA	GLN	A	216	33.689	26.536	24.662	1.00	40.03
1560	C	GLN	A	216	32.649	26.243	25.736	1.00	38.52
1561	O	GLN	A	216	32.207	25.093	25.842	1.00	38.43
1562	CB	GLN	A	216	34.948	25.709	24.953	1.00	42.11
1563	CG	GLN	A	216	36.081	25.871	23.963	1.00	44.52
1564	CD	GLN	A	216	36.980	27.057	24.241	1.00	46.34
1565	OE1	GLN	A	216	36.910	27.707	25.293	1.00	47.64
1566	NE2	GLN	A	216	37.842	27.386	23.279	1.00	46.74
1567	N	ALA	A	217	32.268	27.225	26.536	1.00	36.20
1568	CA	ALA	A	217	31.303	27.017	27.608	1.00	34.50
1569	C	ALA	A	217	29.987	27.715	27.287	1.00	33.15
1570	O	ALA	A	217	28.997	27.578	28.001	1.00	32.25
1571	CB	ALA	A	217	31.880	27.557	28.914	1.00	34.14
1572	N	ALA	A	218	29.996	28.465	26.196	1.00	32.07
1573	CA	ALA	A	218	28.856	29.223	25.721	1.00	31.43
1574	C	ALA	A	218	27.613	28.361	25.529	1.00	31.15
1575	O	ALA	A	218	26.539	28.709	26.018	1.00	31.19

Figure 2-25

1576	CB	ALA	A	218	29.199	29.923	24.407	1.00	30.76
1577	N	SER	A	219	27.771	27.274	24.795	1.00	30.96
1578	CA	SER	A	219	26.679	26.362	24.487	1.00	31.23
1579	C	SER	A	219	26.385	25.476	25.684	1.00	31.50
1580	O	SER	A	219	27.187	24.600	26.008	1.00	30.63
1581	CB	SER	A	219	27.062	25.535	23.257	1.00	31.35
1582	OG	SER	A	219	25.973	24.795	22.745	1.00	31.74
1583	N	ARG	A	220	25.240	25.687	26.343	1.00	32.52
1584	CA	ARG	A	220	24.930	24.859	27.519	1.00	33.84
1585	C	ARG	A	220	23.463	24.496	27.638	1.00	34.32
1586	O	ARG	A	220	22.727	24.975	28.505	1.00	34.48
1587	CB	ARG	A	220	25.426	25.582	28.776	1.00	33.63
1588	CG	ARG	A	220	25.147	27.069	28.796	1.00	34.24
1589	CD	ARG	A	220	25.618	27.735	30.070	1.00	35.88
1590	NE	ARG	A	220	27.023	27.517	30.346	1.00	37.22
1591	CZ	ARG	A	220	27.541	26.815	31.336	1.00	37.40
1592	NH1	ARG	A	220	26.758	26.220	32.219	1.00	37.56
1593	NH2	ARG	A	220	28.863	26.708	31.450	1.00	38.33
1594	N	PRO	A	221	22.988	23.595	26.782	1.00	34.72
1595	CA	PRO	A	221	21.610	23.177	26.771	1.00	35.12
1596	C	PRO	A	221	21.070	22.782	28.127	1.00	36.33
1597	O	PRO	A	221	21.575	21.905	28.822	1.00	36.73
1598	CB	PRO	A	221	21.556	22.019	25.790	1.00	34.23
1599	CG	PRO	A	221	22.935	21.743	25.355	1.00	34.39
1600	CD	PRO	A	221	23.771	22.941	25.702	1.00	34.79
1601	N	TRP	A	222	19.982	23.430	28.537	1.00	37.81
1602	CA	TRP	A	222	19.253	23.204	29.764	1.00	38.35
1603	C	TRP	A	222	19.870	23.783	31.021	1.00	40.00
1604	O	TRP	A	222	19.244	23.803	32.087	1.00	40.39
1605	CB	TRP	A	222	18.989	21.704	29.960	1.00	37.21
1606	CG	TRP	A	222	18.017	21.170	28.940	1.00	36.16
1607	CD1	TRP	A	222	16.705	21.496	28.811	1.00	35.54
1608	CD2	TRP	A	222	18.304	20.213	27.913	1.00	35.39
1609	NE1	TRP	A	222	16.151	20.796	27.769	1.00	35.19
1610	CE2	TRP	A	222	17.111	20.004	27.203	1.00	35.06
1611	CE3	TRP	A	222	19.453	19.511	27.533	1.00	35.46
1612	CZ2	TRP	A	222	17.030	19.127	26.123	1.00	35.14
1613	CZ3	TRP	A	222	19.370	18.638	26.460	1.00	35.39
1614	CH2	TRP	A	222	18.165	18.456	25.770	1.00	35.07
1615	N	ASP	A	223	21.097	24.269	30.942	1.00	41.44
1616	CA	ASP	A	223	21.747	24.939	32.048	1.00	42.07
1617	C	ASP	A	223	21.001	26.228	32.378	1.00	43.35
1618	O	ASP	A	223	20.401	26.868	31.510	1.00	42.75
1619	CB	ASP	A	223	23.201	25.239	31.680	1.00	41.91
1620	CG	ASP	A	223	23.978	25.779	32.868	1.00	42.02
1621	OD1	ASP	A	223</					

Figure 2-26

1639	OE1	GLU	A	225	26.658	31.171	34.461	1.00	52.70
1640	OE2	GLU	A	225	26.323	29.336	35.663	1.00	52.08
1641	N	ARG	A	226	22.030	29.558	30.316	1.00	42.31
1642	CA	ARG	A	226	21.854	29.621	28.870	1.00	40.38
1643	C	ARG	A	226	21.618	31.059	28.409	1.00	38.31
1644	O	ARG	A	226	20.851	31.766	29.076	1.00	38.79
1645	CB	ARG	A	226	20.595	28.839	28.463	1.00	41.11
1646	CG	ARG	A	226	20.733	27.358	28.276	1.00	42.80
1647	CD	ARG	A	226	19.386	26.645	28.252	1.00	44.07
1648	NE	ARG	A	226	18.414	27.281	29.116	1.00	46.50
1649	CZ	ARG	A	226	17.366	26.721	29.696	1.00	47.73
1650	NH1	ARG	A	226	17.078	25.440	29.522	1.00	48.79
1651	NH2	ARG	A	226	16.571	27.446	30.475	1.00	48.31
1652	N	ASP	A	227	22.171	31.480	27.286	1.00	36.03
1653	CA	ASP	A	227	21.891	32.830	26.791	1.00	33.63
1654	C	ASP	A	227	21.674	32.838	25.285	1.00	32.31
1655	O	ASP	A	227	21.554	33.919	24.700	1.00	32.59
1656	CB	ASP	A	227	22.967	33.825	27.192	1.00	32.84
1657	CG	ASP	A	227	24.334	33.499	26.637	1.00	33.33
1658	OD1	ASP	A	227	24.627	32.286	26.529	1.00	34.69
1659	OD2	ASP	A	227	25.120	34.414	26.307	1.00	32.44
1660	N	GLY	A	228	21.550	31.672	24.654	1.00	30.62
1661	CA	GLY	A	228	21.366	31.677	23.188	1.00	28.87
1662	C	GLY	A	228	22.125	30.526	22.548	1.00	27.72
1663	O	GLY	A	228	23.023	29.955	23.172	1.00	28.88
1664	N	PHE	A	229	21.754	30.147	21.330	1.00	25.72
1665	CA	PHE	A	229	22.412	29.027	20.666	1.00	22.79
1666	C	PHE	A	229	23.772	29.488	20.159	1.00	22.85
1667	O	PHE	A	229	24.077	30.672	20.162	1.00	21.95
1668	CB	PHE	A	229	21.550	28.413	19.591	1.00	21.43
1669	CG	PHE	A	229	21.327	29.142	18.316	1.00	20.46
1670	CD1	PHE	A	229	22.236	29.069	17.275	1.00	19.91
1671	CD2	PHE	A	229	20.191	29.920	18.131	1.00	20.66
1672	CE1	PHE	A	229	22.025	29.759	16.087	1.00	19.15
1673	CE2	PHE	A	229	19.969	30.605	16.944	1.00	19.34
1674	CZ	PHE	A	229	20.894	30.517	15.928	1.00	18.75
1675	N	VAL	A	230	24.597	28.526	19.795	1.00	24.11
1676	CA	VAL	A	230	25.926	28.768	19.252	1.00	24.59
1677	C	VAL	A	230	25.972	28.253	17.810	1.00	24.91
1678	O	VAL	A	230	25.540	27.150	17.497	1.00	23.86
1679	CB	VAL	A	230	27.024	28.118	20.106	1.00	24.60
1680	CG1	VAL	A	230	28.392	28.206	19.448	1.00	23.60
1681	CG2	VAL	A	230	27.076	28.781	21.486	1.00	23.95
1682	N	LEU	A	231	26.347	29.141	16.910	1.00	26.19
1683	CA	LEU	A	231	26.347	28.898	15.471	1.00	27.19
1684	C	LEU	A	231	27.458	27.932	15.080	1.00	27.61
1685	O	LEU	A	231	28.575	28.038	15.608	1.00	27.83
1686	CB	LEU	A	231	26.532	30.244	14.786	1.00	27.96
1687	CG	LEU	A	231	26.207	30.468	13.329	1.00	29.21
1688	CD1	LEU	A	231	25.563	29.269	12.659	1.00	29.75
1689	CD2	LEU	A	231	25.315	31.702	13.176	1.00	29.24
1690	N	GLY	A	232	27.171	27.010	14.159	1.00	26.20
1691	CA	GLY	A	232	28.192	26.067	13.714	1.00	24.72
1692	C	GLY	A	232	28.023	25.702	12.248	1.00	23.99
1693	O	GLY	A	232	26.901	25.451	11.800	1.00	24.18
1694	N	ASP	A	233	29.117	25.550	11.512	1.00	23.28
1695	CA	ASP	A	233	29.061	25.134	10.117	1.00	22.60
1696	C	ASP	A	233	29.340	23.637	9.959	1.00	21.54
1697	O	ASP	A	233	29.988	23.027	10.810	1.00	20.87
1698	CB	ASP	A	233	30.079	25.883	9.261	1.00	23.15
1699	CG	ASP	A	233	30.103	27.370	9.485	1.00	24.40
1700	OD1	ASP	A	233	29.054	27.994	9.749	1.00	24.44
1701	OD2	ASP	A	233	31.216	27.933	9.398	1.00	26.06

Figure 2-27

1702	N	GLY	A	234	28.918	23.080	8.825	1.00	20.29
1703	CA	GLY	A	234	29.210	21.686	8.549	1.00	21.48
1704	C	GLY	A	234	28.252	21.018	7.587	1.00	22.09
1705	O	GLY	A	234	27.397	21.642	6.971	1.00	22.10
1706	N	ALA	A	235	28.367	19.694	7.476	1.00	23.04
1707	CA	ALA	A	235	27.488	18.924	6.612	1.00	24.26
1708	C	ALA	A	235	27.550	17.452	7.013	1.00	25.10
1709	O	ALA	A	235	28.601	16.959	7.413	1.00	25.69
1710	CB	ALA	A	235	27.839	19.064	5.141	1.00	24.12
1711	N	GLY	A	236	26.406	16.810	6.904	1.00	25.31
1712	CA	GLY	A	236	26.263	15.399	7.203	1.00	25.96
1713	C	GLY	A	236	25.401	14.764	6.106	1.00	27.84
1714	O	GLY	A	236	24.292	15.232	5.828	1.00	28.18
1715	N	MET	A	237	25.956	13.732	5.480	1.00	27.94
1716	CA	MET	A	237	25.264	13.032	4.412	1.00	28.58
1717	C	MET	A	237	25.021	11.579	4.791	1.00	29.18
1718	O	MET	A	237	25.840	10.946	5.457	1.00	30.25
1719	CB	MET	A	237	26.058	13.121	3.111	1.00	29.09
1720	CG	MET	A	237	26.241	14.540	2.584	1.00	30.84
1721	SD	MET	A	237	24.689	15.275	2.005	1.00	31.49
1722	CE	MET	A	237	23.983	13.854	1.197	1.00	32.58
1723	N	LEU	A	238	23.861	11.059	4.432	1.00	29.03
1724	CA	LEU	A	238	23.455	9.697	4.647	1.00	28.93
1725	C	LEU	A	238	23.154	9.058	3.274	1.00	30.08
1726	O	LEU	A	238	22.641	9.736	2.395	1.00	30.53
1727	CB	LEU	A	238	22.174	9.573	5.445	1.00	29.18
1728	CG	LEU	A	238	21.953	9.963	6.879	1.00	28.28
1729	CD1	LEU	A	238	21.343	8.806	7.674	1.00	28.10
1730	CD2	LEU	A	238	23.203	10.416	7.588	1.00	28.92
1731	N	VAL	A	239	23.389	7.769	3.139	1.00	31.20
1732	CA	VAL	A	239	22.950	7.027	1.966	1.00	31.08
1733	C	VAL	A	239	21.801	6.122	2.442	1.00	31.88
1734	O	VAL	A	239	21.972	5.326	3.365	1.00	31.48
1735	CB	VAL	A	239	24.047	6.189	1.317	1.00	30.98
1736	CG1	VAL	A	239	23.493	5.297	0.207	1.00	30.65
1737	CG2	VAL	A	239	25.150	7.069	0.756	1.00	30.59
1738	N	LEU	A	240	20.614	6.367	1.910	1.00	32.81
1739	CA	LEU	A	240	19.465	5.539	2.267	1.00	34.06
1740	C	LEU	A	240	19.197	4.602	1.091	1.00	35.24
1741	O	LEU	A	240	19.377	5.025	-0.056	1.00	35.94
1742	CB	LEU	A	240	18.233	6.367	2.568	1.00	34.52
1743	CG	LEU	A	240	18.327	7.391	3.694	1.00	34.89
1744	CD1	LEU	A	240	17.392	8.562	3.424	1.00	35.01
1745	CD2	LEU	A	240	18.007	6.741	5.029	1.00	34.67
1746	N	GLU	A	241	18.858	3.355	1.376	1.00	36.34
1747	CA	GLU	A	241	18.549	2.426	0.288	1.00	37.40
1748	C								

Figure 2-28

1765	CA	TYR	A	243	16.528	-3.249	2.295	1.00	47.55
1766	C	TYR	A	243	16.969	-4.314	1.312	1.00	49.06
1767	O	TYR	A	243	18.165	-4.612	1.194	1.00	48.62
1768	CB	TYR	A	243	15.501	-3.828	3.281	1.00	49.37
1769	CG	TYR	A	243	16.082	-4.940	4.129	1.00	51.38
1770	CD1	TYR	A	243	16.964	-4.671	5.162	1.00	51.69
1771	CD2	TYR	A	243	15.741	-6.264	3.873	1.00	52.26
1772	CE1	TYR	A	243	17.492	-5.698	5.921	1.00	52.76
1773	CE2	TYR	A	243	16.261	-7.293	4.635	1.00	52.69
1774	CZ	TYR	A	243	17.141	-7.004	5.652	1.00	52.88
1775	OH	TYR	A	243	17.668	-8.024	6.409	1.00	53.60
1776	N	GLU	A	244	16.023	-4.912	0.584	1.00	50.65
1777	CA	GLU	A	244	16.323	-5.960	-0.383	1.00	51.25
1778	C	GLU	A	244	17.448	-5.559	-1.325	1.00	51.58
1779	O	GLU	A	244	18.371	-6.345	-1.534	1.00	51.59
1780	CB	GLU	A	244	15.091	-6.361	-1.191	1.00	51.54
1781	CG	GLU	A	244	13.925	-6.882	-0.386	1.00	52.35
1782	CD	GLU	A	244	14.242	-8.097	0.454	1.00	53.32
1783	OE1	GLU	A	244	15.188	-8.845	0.125	1.00	53.91
1784	OE2	GLU	A	244	13.535	-8.312	1.464	1.00	53.96
1785	N	HIS	A	245	17.376	-4.358	-1.889	1.00	52.37
1786	CA	HIS	A	245	18.422	-3.872	-2.788	1.00	53.53
1787	C	HIS	A	245	19.776	-3.940	-2.079	1.00	54.72
1788	O	HIS	A	245	20.741	-4.460	-2.619	1.00	54.26
1789	CB	HIS	A	245	18.120	-2.454	-3.239	1.00	53.08
1790	CG	HIS	A	245	19.042	-1.894	-4.277	1.00	52.59
1791	ND1	HIS	A	245	20.337	-1.511	-4.003	1.00	52.62
1792	CD2	HIS	A	245	18.841	-1.610	-5.584	1.00	52.43
1793	CE1	HIS	A	245	20.899	-1.032	-5.096	1.00	52.61
1794	NE2	HIS	A	245	20.012	-1.087	-6.075	1.00	52.66
1795	N	ALA	A	246	19.814	-3.419	-0.859	1.00	56.49
1796	CA	ALA	A	246	20.984	-3.410	-0.006	1.00	58.02
1797	C	ALA	A	246	21.414	-4.832	0.362	1.00	59.33
1798	O	ALA	A	246	22.605	-5.134	0.342	1.00	59.12
1799	CB	ALA	A	246	20.685	-2.632	1.276	1.00	57.55
1800	N	LYS	A	247	20.452	-5.691	0.677	1.00	60.88
1801	CA	LYS	A	247	20.736	-7.079	1.017	1.00	62.53
1802	C	LYS	A	247	21.478	-7.785	-0.112	1.00	63.46
1803	O	LYS	A	247	22.586	-8.299	0.062	1.00	64.16
1804	CB	LYS	A	247	19.444	-7.828	1.336	1.00	62.93
1805	CG	LYS	A	247	19.190	-8.093	2.806	1.00	63.75
1806	CD	LYS	A	247	18.323	-9.329	3.008	1.00	64.65
1807	CE	LYS	A	247	18.834	-10.207	4.137	1.00	65.11
1808	NZ	LYS	A	247	17.770	-11.078	4.710	1.00	65.33
1809	N	LYS	A	248	20.890	-7.806	-1.300	1.00	63.98
1810	CA	LYS	A	248	21.459	-8.440	-2.475	1.00	64.52
1811	C	LYS	A	248	22.870	-7.995	-2.808	1.00	64.22
1812	O	LYS	A	248	23.676	-8.794	-3.305	1.00	64.61
1813	CB	LYS	A	248	20.526	-8.201	-3.673	1.00	65.73
1814	CG	LYS	A	248	21.041	-8.731	-4.997	1.00	67.49
1815	CD	LYS	A	248	19.933	-9.335	-5.847	1.00	68.99
1816	CE	LYS	A	248	19.422	-10.650	-5.279	1.00	69.64
1817	NZ	LYS	A	248	18.013	-10.943	-5.671	1.00	69.80
1818	N	ARG	A	249	23.220	-6.740	-2.582	1.00	63.72
1819	CA	ARG	A	249	24.542	-6.222	-2.893	1.00	63.29
1820	C	ARG	A	249	25.520	-6.419	-1.743	1.00	62.36
1821	O	ARG	A	249	26.712	-6.136	-1.891	1.00	62.39
1822	CB	ARG	A	249	24.449	-4.730	-3.260	1.00	63.82
1823	CG	ARG	A	249	23.678	-3.920	-2.231	1.00	64.36
1824	CD	ARG	A	249	23.874	-2.430	-2.376	1.00	64.71
1825	NE	ARG	A	249	25.279	-2.056	-2.335	1.00	64.93
1826	CZ	ARG	A	249	25.762	-0.961	-1.772	1.00	64.91
1827	NH1	ARG	A	249	24.951	-0.101	-1.182	1.00	64.78

Figure 2-29

1828	NH2	ARG	A	249	27.067	-0.745	-1.812	1.00	65.38
1829	N	GLY	A	250	25.040	-6.911	-0.607	1.00	60.87
1830	CA	GLY	A	250	25.913	-7.131	0.548	1.00	59.90
1831	C	GLY	A	250	26.469	-5.794	1.037	1.00	58.77
1832	O	GLY	A	250	27.666	-5.532	0.986	1.00	58.78
1833	N	ALA	A	251	25.565	-4.945	1.522	1.00	57.41
1834	CA	ALA	A	251	25.944	-3.621	1.977	1.00	55.66
1835	C	ALA	A	251	26.096	-3.568	3.491	1.00	54.72
1836	O	ALA	A	251	25.302	-4.138	4.231	1.00	55.01
1837	CB	ALA	A	251	24.901	-2.602	1.531	1.00	55.46
1838	N	LYS	A	252	27.088	-2.814	3.936	1.00	53.10
1839	CA	LYS	A	252	27.217	-2.428	5.336	1.00	51.33
1840	C	LYS	A	252	25.891	-1.818	5.792	1.00	49.96
1841	O	LYS	A	252	25.612	-0.691	5.346	1.00	50.79
1842	CB	LYS	A	252	28.294	-1.349	5.418	1.00	51.97
1843	CG	LYS	A	252	29.460	-1.544	6.340	1.00	52.61
1844	CD	LYS	A	252	30.208	-0.239	6.593	1.00	53.01
1845	CE	LYS	A	252	30.836	0.346	5.343	1.00	52.98
1846	NZ	LYS	A	252	32.219	-0.157	5.097	1.00	53.69
1847	N	ILE	A	253	25.090	-2.482	6.604	1.00	47.12
1848	CA	ILE	A	253	23.840	-1.881	7.062	1.00	44.71
1849	C	ILE	A	253	24.020	-1.246	8.435	1.00	43.36
1850	O	ILE	A	253	24.012	-1.935	9.462	1.00	44.22
1851	CB	ILE	A	253	22.674	-2.884	7.110	1.00	45.09
1852	CG1	ILE	A	253	22.284	-3.326	5.694	1.00	44.84
1853	CG2	ILE	A	253	21.477	-2.282	7.844	1.00	44.25
1854	CD1	ILE	A	253	20.932	-4.007	5.591	1.00	44.67
1855	N	TYR	A	254	24.049	0.082	8.495	1.00	41.00
1856	CA	TYR	A	254	24.201	0.773	9.772	1.00	38.50
1857	C	TYR	A	254	22.948	0.731	10.628	1.00	37.38
1858	O	TYR	A	254	23.010	0.615	11.853	1.00	38.15
1859	CB	TYR	A	254	24.571	2.235	9.557	1.00	37.33
1860	CG	TYR	A	254	25.979	2.477	9.071	1.00	36.11
1861	CD1	TYR	A	254	26.250	2.657	7.726	1.00	35.30
1862	CD2	TYR	A	254	27.031	2.550	9.972	1.00	35.51
1863	CE1	TYR	A	254	27.538	2.899	7.292	1.00	35.59
1864	CE2	TYR	A	254	28.322	2.787	9.545	1.00	34.81
1865	CZ	TYR	A	254	28.567	2.969	8.209	1.00	35.14
1866	OH	TYR	A	254	29.845	3.209	7.764	1.00	35.01
1867	N	ALA	A	255	21.792	0.886	10.004	1.00	36.44
1868	CA	ALA	A	255	20.536	0.899	10.748	1.00	35.71
1869	C	ALA	A	255	19.367	0.917	9.769	1.00	35.68
1870	O	ALA	A	255	19.573	0.959	8.558	1.00	34.91
1871	CB	ALA	A	255	20.481	2.114	11.662	1.00	35.22
1872	N	GLU	A	256	18.168	0.899	10.321	1.00	36.53
1873	CA	GLU	A	256	16.945	0.951	9.552	1.00	37.42
1874	C	GLU	A	256	16.152	2.209	9.902	1.00	37.04
1875	O	GLU	A	256	15.941	2.490	11.086	1.00	36.85
1876	CB	GLU	A	256	16.054	-0.267	9.831	1.00	39.31
1877	CG	GLU	A	256	15.103	-0.594	8.690	1.00	42.01
1878	CD	GLU	A	256	14.074	-1.643	9.048	1.00	43.86
1879	OE1	GLU	A	256	12.853	-1.395	8.910	1.00	44.65
1880	OE2	GLU	A	256	14.479	-2.750	9.478	1.00	45.17
1881	N	LEU	A	257	15.723	2.931	8.874	1.00	36.43
1882	CA	LEU	A	257	14.882	4.120	9.112	1.00	35.83
1883	C	LEU	A	257	13.456	3.603	9.292	1.00	35.09
1884	O	LEU	A	257	12.950	2.950	8.368	1.00	35.81
1885	CB	LEU	A	257	14.990	5.075	7.952	1.00	36.17
1886	CG	LEU	A	257	14.474	6.497	8.023	1.00	36.62
1887	CD1	LEU	A	257	14.176	6.980	9.428	1.00	36.47
1888	CD2	LEU	A	257	15.503	7.434	7.371	1.00	36.59
1889	N	VAL	A	258	12.898	3.663	10.496	1.00	34.38
1890	CA	VAL	A	258	11.603	3.034	10.719	1.00	34.14

Figure 2-30

1891	C	VAL	A	258	10.495	4.012	11.049	1.00	33.65
1892	O	VAL	A	258	9.349	3.561	11.194	1.00	34.38
1893	CB	VAL	A	258	11.619	1.965	11.845	1.00	34.54
1894	CG1	VAL	A	258	12.689	0.913	11.602	1.00	33.95
1895	CG2	VAL	A	258	11.761	2.594	13.219	1.00	32.70
1896	N	GLY	A	259	10.787	5.287	11.243	1.00	33.01
1897	CA	GLY	A	259	9.718	6.223	11.594	1.00	32.64
1898	C	GLY	A	259	10.094	7.640	11.195	1.00	33.38
1899	O	GLY	A	259	11.260	8.010	11.307	1.00	34.33
1900	N	PHE	A	260	9.104	8.408	10.758	1.00	32.82
1901	CA	PHE	A	260	9.288	9.793	10.342	1.00	31.11
1902	C	PHE	A	260	8.028	10.607	10.608	1.00	30.38
1903	O	PHE	A	260	6.958	10.321	10.062	1.00	30.80
1904	CB	PHE	A	260	9.666	9.859	8.864	1.00	30.74
1905	CG	PHE	A	260	9.673	11.244	8.289	1.00	30.39
1906	CD1	PHE	A	260	10.339	12.272	8.939	1.00	30.56
1907	CD2	PHE	A	260	9.014	11.518	7.103	1.00	30.06
1908	CE1	PHE	A	260	10.344	13.552	8.419	1.00	30.43
1909	CE2	PHE	A	260	9.023	12.791	6.566	1.00	29.90
1910	CZ	PHE	A	260	9.687	13.803	7.227	1.00	30.57
1911	N	GLY	A	261	8.141	11.610	11.470	1.00	29.70
1912	CA	GLY	A	261	7.008	12.434	11.837	1.00	28.92
1913	C	GLY	A	261	7.223	13.919	11.616	1.00	29.15
1914	O	GLY	A	261	8.264	14.502	11.927	1.00	28.06
1915	N	MET	A	262	6.195	14.568	11.075	1.00	29.65
1916	CA	MET	A	262	6.234	16.006	10.832	1.00	30.20
1917	C	MET	A	262	5.070	16.647	11.596	1.00	30.06
1918	O	MET	A	262	4.076	15.969	11.820	1.00	30.13
1919	CB	MET	A	262	6.108	16.345	9.363	1.00	30.45
1920	CG	MET	A	262	7.201	15.870	8.440	1.00	30.83
1921	SD	MET	A	262	6.528	15.370	6.839	1.00	33.07
1922	CE	MET	A	262	6.552	16.931	5.973	1.00	33.59
1923	N	SER	A	263	5.220	17.898	11.968	1.00	30.55
1924	CA	SER	A	263	4.195	18.630	12.684	1.00	31.14
1925	C	SER	A	263	4.371	20.143	12.513	1.00	31.88
1926	O	SER	A	263	5.461	20.618	12.178	1.00	31.41
1927	CB	SER	A	263	4.271	18.315	14.184	1.00	31.36
1928	OG	SER	A	263	5.026	19.356	14.817	1.00	32.23
1929	N	SER	A	264	3.304	20.883	12.800	1.00	32.27
1930	CA	SER	A	264	3.383	22.344	12.751	1.00	33.13
1931	C	SER	A	264	2.953	22.913	14.107	1.00	33.50
1932	O	SER	A	264	2.190	22.277	14.843	1.00	34.89
1933	CB	SER	A	264	2.563	22.928	11.619	1.00	33.19
1934	OG	SER	A	264	3.245	22.889	10.378	1.00	32.30
1935	N	ASP	A	265	3.549	24.024	14.495	1.00	32.03
1936	CA	ASP	A	265	3.310	24.635	15.783	1.00	31.81
1937	C	ASP							

Figure 2-31

1954	CD1	TYR	A	267	1.870	30.187	20.475	1.00	46.70
1955	CD2	TYR	A	267	4.240	30.225	20.194	1.00	46.17
1956	CE1	TYR	A	267	1.997	30.980	21.598	1.00	47.78
1957	CE2	TYR	A	267	4.369	31.016	21.316	1.00	46.66
1958	CZ	TYR	A	267	3.246	31.393	22.012	1.00	47.81
1959	OH	TYR	A	267	3.352	32.177	23.146	1.00	49.51
1960	N	HIS	A	268	4.167	30.890	16.898	1.00	39.39
1961	CA	HIS	A	268	4.985	32.066	16.641	1.00	38.82
1962	C	HIS	A	268	5.976	31.797	15.519	1.00	38.25
1963	O	HIS	A	268	6.275	30.640	15.227	1.00	37.62
1964	CB	HIS	A	268	5.684	32.479	17.942	1.00	38.89
1965	CG	HIS	A	268	6.302	33.838	17.821	1.00	38.92
1966	ND1	HIS	A	268	7.602	34.018	17.404	1.00	39.06
1967	CD2	HIS	A	268	5.784	35.065	18.025	1.00	39.28
1968	CE1	HIS	A	268	7.871	35.309	17.376	1.00	39.76
1969	NE2	HIS	A	268	6.783	35.966	17.743	1.00	40.01
1970	N	MET	A	269	6.475	32.851	14.890	1.00	38.43
1971	CA	MET	A	269	7.351	32.732	13.739	1.00	39.01
1972	C	MET	A	269	8.749	32.275	14.107	1.00	39.15
1973	O	MET	A	269	9.426	31.657	13.275	1.00	39.25
1974	CB	MET	A	269	7.386	34.016	12.910	1.00	38.43
1975	CG	MET	A	269	7.675	35.291	13.655	1.00	38.54
1976	SD	MET	A	269	8.284	36.624	12.597	1.00	39.05
1977	CE	MET	A	269	6.747	37.295	11.973	1.00	38.85
1978	N	THR	A	270	9.206	32.554	15.318	1.00	39.79
1979	CA	THR	A	270	10.544	32.142	15.738	1.00	39.79
1980	C	THR	A	270	10.491	31.386	17.061	1.00	39.73
1981	O	THR	A	270	11.262	30.461	17.286	1.00	40.16
1982	CB	THR	A	270	11.500	33.336	15.909	1.00	39.47
1983	OG1	THR	A	270	10.849	34.378	16.650	1.00	38.86
1984	CG2	THR	A	270	11.946	33.850	14.549	1.00	39.41
1985	N	SER	A	271	9.562	31.784	17.912	1.00	39.92
1986	CA	SER	A	271	9.368	31.191	19.218	1.00	40.15
1987	C	SER	A	271	8.529	29.923	19.208	1.00	39.41
1988	O	SER	A	271	7.519	29.833	18.522	1.00	38.39
1989	CB	SER	A	271	8.655	32.218	20.122	1.00	40.93
1990	OG	SER	A	271	9.597	32.892	20.930	1.00	42.94
1991	N	PRO	A	272	8.916	28.967	20.033	1.00	39.55
1992	CA	PRO	A	272	8.149	27.755	20.264	1.00	39.89
1993	C	PRO	A	272	7.144	27.989	21.382	1.00	40.70
1994	O	PRO	A	272	7.253	28.945	22.155	1.00	40.74
1995	CB	PRO	A	272	9.213	26.763	20.710	1.00	39.54
1996	CG	PRO	A	272	10.251	27.585	21.378	1.00	39.69
1997	CD	PRO	A	272	10.104	29.011	20.924	1.00	39.50
1998	N	PRO	A	273	6.128	27.155	21.451	1.00	41.57
1999	CA	PRO	A	273	5.155	27.209	22.529	1.00	41

Figure 2-32

2017	O	ASN	A	275	5.181	21.540	25.870	1.00	45.50
2018	CB	ASN	A	275	2.792	23.832	25.226	1.00	48.36
2019	CG	ASN	A	275	1.786	22.757	25.501	1.00	50.56
2020	OD1	ASN	A	275	0.610	23.052	25.746	1.00	51.89
2021	ND2	ASN	A	275	2.222	21.499	25.461	1.00	51.68
2022	N	GLY	A	276	5.404	22.926	24.142	1.00	43.78
2023	CA	GLY	A	276	6.162	21.984	23.332	1.00	41.18
2024	C	GLY	A	276	5.229	21.052	22.558	1.00	39.94
2025	O	GLY	A	276	5.630	19.999	22.057	1.00	38.60
2026	N	ALA	A	277	3.960	21.444	22.429	1.00	38.88
2027	CA	ALA	A	277	2.943	20.651	21.765	1.00	38.13
2028	C	ALA	A	277	3.282	20.243	20.338	1.00	37.49
2029	O	ALA	A	277	2.921	19.138	19.911	1.00	37.45
2030	CB	ALA	A	277	1.602	21.380	21.780	1.00	37.64
2031	N	GLY	A	278	3.871	21.144	19.562	1.00	36.32
2032	CA	GLY	A	278	4.257	20.831	18.183	1.00	34.59
2033	C	GLY	A	278	5.357	19.776	18.211	1.00	33.11
2034	O	GLY	A	278	5.263	18.743	17.545	1.00	32.66
2035	N	ALA	A	279	6.362	20.011	19.051	1.00	31.37
2036	CA	ALA	A	279	7.431	19.025	19.215	1.00	31.33
2037	C	ALA	A	279	6.857	17.681	19.660	1.00	31.17
2038	O	ALA	A	279	7.231	16.611	19.159	1.00	31.33
2039	CB	ALA	A	279	8.444	19.546	20.212	1.00	31.56
2040	N	ALA	A	280	5.884	17.714	20.562	1.00	30.93
2041	CA	ALA	A	280	5.212	16.518	21.041	1.00	31.18
2042	C	ALA	A	280	4.505	15.758	19.932	1.00	31.56
2043	O	ALA	A	280	4.626	14.536	19.788	1.00	31.58
2044	CB	ALA	A	280	4.227	16.911	22.141	1.00	30.59
2045	N	LEU	A	281	3.781	16.482	19.078	1.00	31.84
2046	CA	LEU	A	281	2.989	15.831	18.031	1.00	32.50
2047	C	LEU	A	281	3.840	15.238	16.924	1.00	32.77
2048	O	LEU	A	281	3.402	14.330	16.205	1.00	32.06
2049	CB	LEU	A	281	1.958	16.823	17.508	1.00	33.11
2050	CG	LEU	A	281	1.157	16.429	16.271	1.00	34.64
2051	CD1	LEU	A	281	0.256	15.241	16.556	1.00	33.87
2052	CD2	LEU	A	281	0.351	17.623	15.767	1.00	34.77
2053	N	ALA	A	282	5.072	15.723	16.774	1.00	32.69
2054	CA	ALA	A	282	5.988	15.209	15.765	1.00	31.83
2055	C	ALA	A	282	6.667	13.936	16.256	1.00	31.20
2056	O	ALA	A	282	6.953	13.060	15.448	1.00	29.68
2057	CB	ALA	A	282	7.022	16.256	15.397	1.00	32.01
2058	N	MET	A	283	6.927	13.865	17.571	1.00	31.55
2059	CA	MET	A	283	7.522	12.619	18.101	1.00	32.09
2060	C	MET	A	283	6.415	11.558	18.038	1.00	32.78
2061	O	MET	A	283	6.510	10.526	17.386	1.00	32.13
2062	CB	MET	A	283	8.041	12.793	19.507	1.00	31.89
2									

Figure 2-33

2080	CA	ALA	A	286	6.964	9.362	14.285	1.00	34.55
2081	C	ALA	A	286	6.742	7.970	14.874	1.00	35.42
2082	O	ALA	A	286	6.960	6.935	14.264	1.00	34.04
2083	CB	ALA	A	286	8.268	9.936	14.818	1.00	33.75
2084	N	LEU	A	287	6.321	7.995	16.143	1.00	37.17
2085	CA	LEU	A	287	6.018	6.780	16.884	1.00	38.32
2086	C	LEU	A	287	4.957	5.967	16.164	1.00	39.73
2087	O	LEU	A	287	5.158	4.784	15.877	1.00	38.69
2088	CB	LEU	A	287	5.600	7.154	18.313	1.00	37.88
2089	CG	LEU	A	287	6.795	7.426	19.249	1.00	37.80
2090	CD1	LEU	A	287	6.334	7.877	20.616	1.00	37.05
2091	CD2	LEU	A	287	7.683	6.190	19.347	1.00	37.58
2092	N	ARG	A	288	3.851	6.632	15.806	1.00	41.38
2093	CA	ARG	A	288	2.769	5.969	15.083	1.00	42.96
2094	C	ARG	A	288	3.269	5.379	13.774	1.00	42.65
2095	O	ARG	A	288	3.015	4.219	13.465	1.00	42.61
2096	CB	ARG	A	288	1.613	6.940	14.836	1.00	45.04
2097	CG	ARG	A	288	0.425	6.321	14.128	1.00	48.66
2098	CD	ARG	A	288	-0.811	7.210	14.128	1.00	51.29
2099	NE	ARG	A	288	-0.651	8.364	13.243	1.00	53.75
2100	CZ	ARG	A	288	-0.499	9.617	13.668	1.00	54.99
2101	NH1	ARG	A	288	-0.514	9.916	14.964	1.00	54.93
2102	NH2	ARG	A	288	-0.326	10.579	12.762	1.00	56.01
2103	N	ASP	A	289	4.067	6.129	13.025	1.00	42.95
2104	CA	ASP	A	289	4.620	5.710	11.751	1.00	42.81
2105	C	ASP	A	289	5.494	4.477	11.897	1.00	43.26
2106	O	ASP	A	289	5.539	3.627	11.010	1.00	43.44
2107	CB	ASP	A	289	5.428	6.850	11.122	1.00	43.06
2108	CG	ASP	A	289	5.762	6.635	9.663	1.00	43.34
2109	OD1	ASP	A	289	6.926	6.875	9.262	1.00	43.42
2110	OD2	ASP	A	289	4.871	6.222	8.888	1.00	43.16
2111	N	ALA	A	290	6.219	4.383	13.006	1.00	44.10
2112	CA	ALA	A	290	7.082	3.243	13.279	1.00	44.21
2113	C	ALA	A	290	6.287	2.108	13.921	1.00	44.87
2114	O	ALA	A	290	6.659	0.944	13.787	1.00	45.98
2115	CB	ALA	A	290	8.234	3.653	14.178	1.00	43.78
2116	N	GLY	A	291	5.218	2.444	14.636	1.00	44.81
2117	CA	GLY	A	291	4.362	1.476	15.281	1.00	44.46
2118	C	GLY	A	291	4.864	1.013	16.634	1.00	44.95
2119	O	GLY	A	291	4.471	-0.051	17.128	1.00	45.58
2120	N	ILE	A	292	5.742	1.778	17.273	1.00	44.88
2121	CA	ILE	A	292	6.300	1.395	18.562	1.00	44.50
2122	C	ILE	A	292	5.816	2.343	19.650	1.00	45.65
2123	O	ILE	A	292	5.155	3.335	19.342	1.00	46.14
2124	CB	ILE	A	292	7.833	1.360	18.544	1.00	43.75
2125	CG1	ILE	A	292	8.408	2.772	18.452	1.00	43.53
2126	CG2	ILE	A	292	8.345				

Figure 2-34

2143	CA	SER	A	295	9.257	3.037	26.133	1.00	47.63
2144	C	SER	A	295	10.346	2.265	25.410	1.00	46.97
2145	O	SER	A	295	11.303	1.793	26.057	1.00	47.56
2146	CB	SER	A	295	8.340	2.003	26.837	1.00	48.01
2147	OG	SER	A	295	8.027	0.966	25.905	1.00	48.28
2148	N	GLN	A	296	10.256	2.092	24.102	1.00	45.19
2149	CA	GLN	A	296	11.275	1.355	23.359	1.00	44.36
2150	C	GLN	A	296	12.408	2.264	22.917	1.00	42.95
2151	O	GLN	A	296	13.471	1.798	22.505	1.00	42.77
2152	CB	GLN	A	296	10.617	0.635	22.180	1.00	45.62
2153	CG	GLN	A	296	9.237	0.075	22.532	1.00	46.57
2154	CD	GLN	A	296	8.730	-0.897	21.494	1.00	47.79
2155	OE1	GLN	A	296	7.551	-0.881	21.125	1.00	48.74
2156	NE2	GLN	A	296	9.609	-1.763	21.001	1.00	48.30
2157	N	ILE	A	297	12.205	3.573	23.038	1.00	41.44
2158	CA	ILE	A	297	13.219	4.559	22.695	1.00	39.95
2159	C	ILE	A	297	14.281	4.624	23.787	1.00	38.41
2160	O	ILE	A	297	14.009	4.967	24.934	1.00	37.64
2161	CB	ILE	A	297	12.625	5.963	22.469	1.00	40.09
2162	CG1	ILE	A	297	11.659	5.978	21.279	1.00	39.62
2163	CG2	ILE	A	297	13.728	6.994	22.250	1.00	39.76
2164	CD1	ILE	A	297	12.247	5.455	19.990	1.00	39.49
2165	N	GLY	A	298	15.515	4.307	23.421	1.00	37.84
2166	CA	GLY	A	298	16.599	4.327	24.404	1.00	37.21
2167	C	GLY	A	298	17.183	5.719	24.557	1.00	37.35
2168	O	GLY	A	298	17.381	6.216	25.665	1.00	37.77
2169	N	TYR	A	299	17.447	6.354	23.420	1.00	37.03
2170	CA	TYR	A	299	18.092	7.654	23.391	1.00	35.98
2171	C	TYR	A	299	17.388	8.622	22.447	1.00	35.82
2172	O	TYR	A	299	17.030	8.314	21.312	1.00	35.55
2173	CB	TYR	A	299	19.551	7.463	22.983	1.00	36.16
2174	CG	TYR	A	299	20.319	8.708	22.633	1.00	36.96
2175	CD1	TYR	A	299	20.929	8.828	21.390	1.00	37.22
2176	CD2	TYR	A	299	20.456	9.757	23.535	1.00	37.10
2177	CE1	TYR	A	299	21.648	9.957	21.048	1.00	37.84
2178	CE2	TYR	A	299	21.165	10.893	23.204	1.00	37.79
2179	CZ	TYR	A	299	21.770	10.981	21.966	1.00	38.60
2180	OH	TYR	A	299	22.504	12.096	21.627	1.00	39.51
2181	N	VAL	A	300	17.222	9.841	22.938	1.00	34.63
2182	CA	VAL	A	300	16.664	10.948	22.185	1.00	33.18
2183	C	VAL	A	300	17.784	11.965	21.929	1.00	32.63
2184	O	VAL	A	300	18.255	12.605	22.871	1.00	32.19
2185	CB	VAL	A	300	15.524	11.660	22.938	1.00	32.62
2186	CG1	VAL	A	300	15.214	13.020	22.333	1.00	32.40
2187	CG2	VAL	A	300	14.269	10.800	22.975	1.00	32.13
2188	N	ASN	A	301	18.193	12.099	20.675	1.00	32.15
2189	CA	ASN	A	301	19.069	13.226	20.309	1.00	31.41
2190	C	ASN	A	301	18.178	14.464	20.181	1.00	30.53
2191	O	ASN	A	301	17.442	14.640	19.215	1.00	31.07
2192	CB	ASN	A	301	19.859	12.951	19.048	1.00	31.30
2193	CG	ASN	A	301	20.806	14.085	18.713	1.00	31.98
2194	OD1	ASN	A	301	21.995	14.005	19.010	1.00	31.87
2195	ND2	ASN	A	301	20.263	15.136	18.093	1.00	32.95
2196	N	ALA	A	302	18.200	15.291	21.205	1.00	29.64
2197	CA	ALA	A	302	17.376	16.466	21.312	1.00	29.90
2198	C	ALA	A	302	17.724	17.596	20.361	1.00	29.88
2199	O	ALA	A	302	18.820	17.710	19.818	1.00	30.09
2200	CB	ALA	A	302	17.484	17.001	22.755	1.00	29.38
2201	N	HIS	A	303	16.747	18.500	20.201	1.00	29.39
2202	CA	HIS	A	303	17.001	19.687	19.382	1.00	29.72
2203	C	HIS	A	303	17.906	20.605	20.225	1.00	29.85
2204	O	HIS	A	303	18.944	21.062	19.777	1.00	29.00
2205	CB	HIS	A	303	15.719	20.388	18.976	1.00	29.67

Figure 2-35

2206	CG	HIS	A	303	15.963	21.570	18.080	1.00	29.65
2207	ND1	HIS	A	303	16.740	21.478	16.942	1.00	30.47
2208	CD2	HIS	A	303	15.552	22.850	18.160	1.00	29.32
2209	CE1	HIS	A	303	16.792	22.660	16.355	1.00	30.67
2210	NE2	HIS	A	303	16.084	23.516	17.084	1.00	30.18
2211	N	GLY	A	304	17.545	20.716	21.499	1.00	30.19
2212	CA	GLY	A	304	18.260	21.378	22.551	1.00	31.04
2213	C	GLY	A	304	19.387	22.299	22.113	1.00	30.87
2214	O	GLY	A	304	20.568	21.962	22.172	1.00	30.26
2215	N	THR	A	305	19.016	23.502	21.704	1.00	30.59
2216	CA	THR	A	305	19.924	24.486	21.163	1.00	30.95
2217	C	THR	A	305	20.526	25.444	22.160	1.00	30.62
2218	O	THR	A	305	21.218	26.374	21.730	1.00	31.05
2219	CB	THR	A	305	19.167	25.300	20.073	1.00	31.44
2220	OG1	THR	A	305	18.143	26.079	20.709	1.00	32.41
2221	CG2	THR	A	305	18.511	24.357	19.074	1.00	30.77
2222	N	SER	A	306	20.310	25.280	23.448	1.00	30.65
2223	CA	SER	A	306	20.823	26.156	24.492	1.00	29.52
2224	C	SER	A	306	20.129	27.510	24.521	1.00	29.40
2225	O	SER	A	306	20.713	28.556	24.800	1.00	28.21
2226	CB	SER	A	306	22.333	26.315	24.382	1.00	29.55
2227	OG	SER	A	306	22.887	26.873	25.564	1.00	29.38
2228	N	THR	A	307	18.828	27.513	24.218	1.00	30.00
2229	CA	THR	A	307	18.054	28.750	24.287	1.00	30.62
2230	C	THR	A	307	17.049	28.601	25.429	1.00	31.06
2231	O	THR	A	307	16.500	27.519	25.623	1.00	30.43
2232	CB	THR	A	307	17.330	29.115	22.986	1.00	29.95
2233	OG1	THR	A	307	16.320	28.137	22.714	1.00	29.62
2234	CG2	THR	A	307	18.318	29.199	21.834	1.00	29.18
2235	N	PRO	A	308	16.948	29.632	26.249	1.00	32.42
2236	CA	PRO	A	308	16.079	29.618	27.413	1.00	33.00
2237	C	PRO	A	308	14.725	29.019	27.109	1.00	34.60
2238	O	PRO	A	308	14.429	27.899	27.560	1.00	36.16
2239	CB	PRO	A	308	15.998	31.083	27.808	1.00	32.75
2240	CG	PRO	A	308	17.304	31.659	27.359	1.00	32.45
2241	CD	PRO	A	308	17.600	30.954	26.056	1.00	32.33
2242	N	ALA	A	309	13.936	29.674	26.262	1.00	35.22
2243	CA	ALA	A	309	12.602	29.191	25.929	1.00	35.74
2244	C	ALA	A	309	12.598	27.867	25.185	1.00	35.62
2245	O	ALA	A	309	11.768	26.998	25.490	1.00	36.25
2246	CB	ALA	A	309	11.839	30.245	25.132	1.00	36.27
2247	N	GLY	A	310	13.473	27.703	24.205	1.00	35.30
2248	CA	GLY	A	310	13.536	26.509	23.394	1.00	34.58
2249	C	GLY	A	310	13.761	25.233	24.178	1.00	35.19
2250	O	GLY	A	310	13.020	24.257	24.002	1.00	34.63
2251	N	ASP	A	311	14.748	25.228	25.076	1.00	36.16
2252	CA	ASP	A	311	15.095	24.027	25.837	1.00	37.35
2253	C	ASP	A	311	13.984	23.622	26.798	1.00	37.28
2254	O	ASP	A	311	13.703	22.442	26.979	1.00	35.57
2255	CB	ASP	A	311	16.425	24.187	26.566	1.00	38.20
2256	CG	ASP	A	311	17.609	24.388	25.642	1.00	39.32
2257	OD1	ASP	A	311	18.776	24.372	26.101	1.00	38.85
2258	OD2	ASP	A	311	17.397	24.571	24.423	1.00	40.40
2259	N	LYS	A	312	13.300	24.604	27.377	1.00	38.66
2260	CA	LYS	A	312	12.173	24.347	28.260	1.00	39.64
2261	C	LYS	A	312	11.110	23.515	27.545	1.00	39.36
2262	O	LYS	A	312	10.686	22.467	28.007	1.00	39.26
2263	CB	LYS	A	312	11.532	25.663	28.693	1.00	41.64
2264	CG	LYS	A	312	12.133	26.320	29.920	1.00	43.75
2265	CD	LYS	A	312	11.035	26.838	30.841	1.00	45.48
2266	CE	LYS	A	312	11.461	28.114	31.550	1.00	47.04
2267	NZ	LYS	A	312	10.296	28.741	32.255	1.00	48.24
2268	N	ALA	A	313	10.680	24.032	26.398	1.00	39.30

Figure 2-36

2269	CA	ALA	A	313	9.625	23.450	25.595	1.00	38.76
2270	C	ALA	A	313	9.893	22.012	25.216	1.00	39.23
2271	O	ALA	A	313	9.032	21.158	25.441	1.00	40.34
2272	CB	ALA	A	313	9.401	24.290	24.340	1.00	38.69
2273	N	GLU	A	314	11.061	21.713	24.651	1.00	39.89
2274	CA	GLU	A	314	11.354	20.344	24.246	1.00	40.45
2275	C	GLU	A	314	11.322	19.373	25.418	1.00	40.84
2276	O	GLU	A	314	10.768	18.279	25.320	1.00	40.97
2277	CB	GLU	A	314	12.721	20.240	23.564	1.00	40.99
2278	CG	GLU	A	314	12.961	18.830	23.011	1.00	40.54
2279	CD	GLU	A	314	14.188	18.798	22.132	1.00	40.81
2280	OE1	GLU	A	314	14.953	19.783	22.149	1.00	40.94
2281	OE2	GLU	A	314	14.361	17.791	21.423	1.00	41.62
2282	N	ALA	A	315	11.963	19.767	26.514	1.00	41.04
2283	CA	ALA	A	315	11.937	18.989	27.740	1.00	41.54
2284	C	ALA	A	315	10.495	18.632	28.093	1.00	41.87
2285	O	ALA	A	315	10.175	17.464	28.313	1.00	41.76
2286	CB	ALA	A	315	12.588	19.759	28.877	1.00	41.38
2287	N	GLN	A	316	9.621	19.640	28.103	1.00	42.34
2288	CA	GLN	A	316	8.217	19.395	28.399	1.00	43.86
2289	C	GLN	A	316	7.595	18.404	27.423	1.00	44.27
2290	O	GLN	A	316	6.988	17.400	27.803	1.00	43.96
2291	CB	GLN	A	316	7.412	20.695	28.386	1.00	44.58
2292	CG	GLN	A	316	5.971	20.493	28.849	1.00	46.52
2293	CD	GLN	A	316	5.893	20.074	30.312	1.00	47.74
2294	OE1	GLN	A	316	6.524	20.669	31.190	1.00	47.58
2295	NE2	GLN	A	316	5.130	19.006	30.546	1.00	47.69
2296	N	ALA	A	317	7.864	18.596	26.130	1.00	44.25
2297	CA	ALA	A	317	7.349	17.688	25.118	1.00	44.89
2298	C	ALA	A	317	7.812	16.258	25.346	1.00	44.92
2299	O	ALA	A	317	7.103	15.311	24.979	1.00	44.45
2300	CB	ALA	A	317	7.760	18.188	23.734	1.00	45.79
2301	N	VAL	A	318	9.008	16.071	25.897	1.00	45.09
2302	CA	VAL	A	318	9.525	14.735	26.187	1.00	45.96
2303	C	VAL	A	318	8.773	14.126	27.372	1.00	46.69
2304	O	VAL	A	318	8.442	12.943	27.383	1.00	46.39
2305	CB	VAL	A	318	11.038	14.753	26.459	1.00	45.52
2306	CG1	VAL	A	318	11.526	13.458	27.096	1.00	45.04
2307	CG2	VAL	A	318	11.806	15.009	25.166	1.00	44.92
2308	N	LYS	A	319	8.439	14.958	28.352	1.00	47.66
2309	CA	LYS	A	319	7.685	14.521	29.517	1.00	49.06
2310	C	LYS	A	319	6.271	14.119	29.128	1.00	49.78
2311	O	LYS	A	319	5.722	13.163	29.680	1.00	50.92
2312	CB	LYS	A	319	7.689	15.604	30.598	1.00	49.56
2313	CG	LYS	A	319	9.083	15.838	31.176	1.00	50.90
2314	CD	LYS	A	319	9.067	16.783	32		

Figure 2-37

2332	N	PHE	A	322	7.062	10.686	26.764	1.00	55.32
2333	CA	PHE	A	322	7.623	9.536	27.482	1.00	57.01
2334	C	PHE	A	322	6.854	9.233	28.751	1.00	58.22
2335	O	PHE	A	322	6.709	8.063	29.131	1.00	58.09
2336	CB	PHE	A	322	9.129	9.740	27.695	1.00	56.37
2337	CG	PHE	A	322	9.837	9.510	26.375	1.00	56.26
2338	CD1	PHE	A	322	9.909	10.521	25.438	1.00	56.23
2339	CD2	PHE	A	322	10.364	8.269	26.073	1.00	56.06
2340	CE1	PHE	A	322	10.527	10.306	24.219	1.00	56.27
2341	CE2	PHE	A	322	10.981	8.052	24.857	1.00	56.46
2342	CZ	PHE	A	322	11.063	9.069	23.926	1.00	56.24
2343	N	GLY	A	323	6.262	10.257	29.358	1.00	59.40
2344	CA	GLY	A	323	5.449	10.098	30.548	1.00	61.56
2345	C	GLY	A	323	6.205	9.479	31.715	1.00	63.08
2346	O	GLY	A	323	7.035	10.135	32.346	1.00	62.72
2347	N	GLU	A	324	5.911	8.211	31.997	1.00	64.65
2348	CA	GLU	A	324	6.532	7.504	33.112	1.00	66.18
2349	C	GLU	A	324	7.932	7.025	32.757	1.00	65.94
2350	O	GLU	A	324	8.799	6.936	33.631	1.00	66.15
2351	CB	GLU	A	324	5.653	6.337	33.561	1.00	67.61
2352	CG	GLU	A	324	4.724	6.673	34.715	1.00	69.11
2353	CD	GLU	A	324	3.266	6.766	34.309	1.00	70.22
2354	OE1	GLU	A	324	2.919	7.668	33.508	1.00	70.44
2355	OE2	GLU	A	324	2.459	5.940	34.799	1.00	70.43
2356	N	ALA	A	325	8.170	6.761	31.475	1.00	65.16
2357	CA	ALA	A	325	9.469	6.309	31.002	1.00	64.72
2358	C	ALA	A	325	10.416	7.477	30.754	1.00	64.29
2359	O	ALA	A	325	11.565	7.276	30.360	1.00	63.88
2360	CB	ALA	A	325	9.326	5.470	29.739	1.00	64.73
2361	N	ALA	A	326	9.977	8.690	31.052	1.00	63.99
2362	CA	ALA	A	326	10.745	9.905	30.917	1.00	63.96
2363	C	ALA	A	326	12.013	9.906	31.759	1.00	64.59
2364	O	ALA	A	326	12.982	10.590	31.423	1.00	65.46
2365	CB	ALA	A	326	9.892	11.111	31.296	1.00	63.23
2366	N	SER	A	327	12.034	9.169	32.856	1.00	64.91
2367	CA	SER	A	327	13.195	9.076	33.724	1.00	64.87
2368	C	SER	A	327	14.168	8.006	33.253	1.00	64.31
2369	O	SER	A	327	15.363	8.062	33.553	1.00	65.08
2370	CB	SER	A	327	12.725	8.745	35.152	1.00	65.49
2371	OG	SER	A	327	11.692	7.767	35.086	1.00	65.92
2372	N	ARG	A	328	13.663	7.014	32.526	1.00	63.15
2373	CA	ARG	A	328	14.520	5.936	32.040	1.00	61.76
2374	C	ARG	A	328	15.101	6.250	30.671	1.00	59.76
2375	O	ARG	A	328	16.033	5.564	30.233	1.00	60.32
2376	CB	ARG	A	328	13.764	4.609	32.025	1.00	62.86
2377	CG	ARG	A	328	12.866	4.373	30.827	1.00	64.26
2378	CD	ARG	A	328	11.855	3.269	31.095	1.00	65.68
2379	NE	ARG	A	328	11.950	2.167	30.144	1.00	66.47
2380	CZ	ARG	A	328	11.064	1.187	30.020	1.00	66.85
2381	NH1	ARG	A	328	9.983	1.158	30.792	1.00	67.11
2382	NH2	ARG	A	328	11.246	0.229	29.119	1.00	67.06
2383	N	VAL	A	329	14.570	7.262	29.985	1.00	56.58
2384	CA	VAL	A	329	15.070	7.594	28.651	1.00	52.91
2385	C	VAL	A	329	16.235	8.569	28.713	1.00	51.13
2386	O	VAL	A	329	16.259	9.466	29.550	1.00	50.77
2387	CB	VAL	A	329	13.964	8.144	27.740	1.00	52.48
2388	CG1	VAL	A	329	13.541	9.544	28.160	1.00	51.82
2389	CG2	VAL	A	329	14.411	8.119	26.284	1.00	51.86
2390	N	LEU	A	330	17.217	8.350	27.844	1.00	48.78
2391	CA	LEU	A	330	18.386	9.205	27.748	1.00	46.67
2392	C	LEU	A	330	18.182	10.298	26.701	1.00	45.85
2393	O	LEU	A	330	17.791	10.038	25.560	1.00	45.82
2394	CB	LEU	A	330	19.627	8.379	27.404	1.00	46.55

Figure 2-38

2395	CG	LEU	A	330	20.032	7.297	28.410	1.00	46.63
2396	CD1	LEU	A	330	21.221	6.501	27.896	1.00	46.07
2397	CD2	LEU	A	330	20.345	7.902	29.769	1.00	45.97
2398	N	VAL	A	331	18.358	11.547	27.118	1.00	43.84
2399	CA	VAL	A	331	18.211	12.702	26.266	1.00	42.46
2400	C	VAL	A	331	19.460	13.580	26.316	1.00	41.99
2401	O	VAL	A	331	19.603	14.358	27.267	1.00	41.78
2402	CB	VAL	A	331	17.022	13.610	26.674	1.00	42.13
2403	CG1	VAL	A	331	16.686	14.548	25.519	1.00	41.88
2404	CG2	VAL	A	331	15.797	12.845	27.111	1.00	41.37
2405	N	SER	A	332	20.281	13.610	25.269	1.00	41.05
2406	CA	SER	A	332	21.423	14.534	25.294	1.00	39.11
2407	C	SER	A	332	21.364	15.492	24.113	1.00	38.45
2408	O	SER	A	332	20.643	15.253	23.151	1.00	38.77
2409	CB	SER	A	332	22.754	13.797	25.309	1.00	38.87
2410	OG	SER	A	332	22.976	13.032	24.140	1.00	38.04
2411	N	SER	A	333	22.152	16.557	24.185	1.00	37.37
2412	CA	SER	A	333	22.327	17.480	23.081	1.00	35.80
2413	C	SER	A	333	23.808	17.578	22.713	1.00	35.02
2414	O	SER	A	333	24.608	18.160	23.448	1.00	34.17
2415	CB	SER	A	333	21.803	18.883	23.391	1.00	35.80
2416	OG	SER	A	333	22.173	19.787	22.353	1.00	34.77
2417	N	THR	A	334	24.153	17.125	21.506	1.00	33.66
2418	CA	THR	A	334	25.523	17.226	21.031	1.00	32.68
2419	C	THR	A	334	25.890	18.626	20.566	1.00	31.79
2420	O	THR	A	334	27.042	18.855	20.175	1.00	32.24
2421	CB	THR	A	334	25.794	16.248	19.874	1.00	33.55
2422	OG1	THR	A	334	24.632	16.210	19.035	1.00	35.08
2423	CG2	THR	A	334	26.091	14.854	20.395	1.00	33.98
2424	N	LYS	A	335	24.966	19.571	20.620	1.00	29.86
2425	CA	LYS	A	335	25.130	20.954	20.255	1.00	28.11
2426	C	LYS	A	335	25.909	21.722	21.323	1.00	28.33
2427	O	LYS	A	335	26.403	22.833	21.112	1.00	28.49
2428	CB	LYS	A	335	23.766	21.632	20.065	1.00	27.41
2429	CG	LYS	A	335	22.985	21.211	18.848	1.00	26.22
2430	CD	LYS	A	335	21.797	22.117	18.573	1.00	25.45
2431	CE	LYS	A	335	21.096	21.719	17.274	1.00	24.18
2432	NZ	LYS	A	335	20.513	20.357	17.370	1.00	22.35
2433	N	SER	A	336	26.063	21.085	22.485	1.00	27.13
2434	CA	SER	A	336	26.898	21.586	23.553	1.00	26.20
2435	C	SER	A	336	28.357	21.641	23.098	1.00	25.15
2436	O	SER	A	336	29.092	22.541	23.491	1.00	24.26
2437	CB	SER	A	336	26.778	20.723	24.803	1.00	26.48
2438	OG	SER	A	336	26.951	19.355	24.499	1.00	26.89
2439	N	MET	A	337	28.738	20.692	22.253	1.00	24.47
2440	CA	MET	A	337	30.088				

Figure 2-39

2458	N	HIS	A	340	25.078	24.779	16.805	1.00	20.63
2459	CA	HIS	A	340	23.911	24.536	15.968	1.00	21.54
2460	C	HIS	A	340	24.257	24.569	14.493	1.00	21.15
2461	O	HIS	A	340	24.500	25.668	13.973	1.00	21.62
2462	CB	HIS	A	340	22.858	25.630	16.248	1.00	23.15
2463	CG	HIS	A	340	21.477	25.188	15.873	1.00	24.70
2464	ND1	HIS	A	340	21.254	24.220	14.915	1.00	25.46
2465	CD2	HIS	A	340	20.258	25.566	16.319	1.00	24.88
2466	CE1	HIS	A	340	19.955	24.014	14.797	1.00	25.60
2467	NE2	HIS	A	340	19.332	24.819	15.640	1.00	25.55
2468	N	LEU	A	341	24.136	23.463	13.765	1.00	21.78
2469	CA	LEU	A	341	24.425	23.446	12.332	1.00	21.51
2470	C	LEU	A	341	23.246	23.864	11.455	1.00	20.67
2471	O	LEU	A	341	23.264	23.596	10.245	1.00	20.80
2472	CB	LEU	A	341	24.939	22.111	11.840	1.00	22.08
2473	CG	LEU	A	341	26.253	21.519	12.279	1.00	23.06
2474	CD1	LEU	A	341	27.036	20.962	11.093	1.00	22.21
2475	CD2	LEU	A	341	27.124	22.487	13.058	1.00	23.72
2476	N	LEU	A	342	22.235	24.517	12.005	1.00	19.56
2477	CA	LEU	A	342	21.091	24.989	11.221	1.00	18.26
2478	C	LEU	A	342	20.559	23.973	10.240	1.00	18.01
2479	O	LEU	A	342	20.095	22.884	10.652	1.00	18.33
2480	CB	LEU	A	342	21.537	26.296	10.539	1.00	17.17
2481	CG	LEU	A	342	22.146	27.319	11.515	1.00	16.80
2482	CD1	LEU	A	342	22.711	28.519	10.799	1.00	16.76
2483	CD2	LEU	A	342	21.099	27.764	12.537	1.00	17.23
2484	N	GLY	A	343	20.749	24.167	8.940	1.00	16.41
2485	CA	GLY	A	343	20.241	23.256	7.937	1.00	15.90
2486	C	GLY	A	343	20.886	21.889	7.985	1.00	17.08
2487	O	GLY	A	343	20.296	20.916	7.502	1.00	18.05
2488	N	ALA	A	344	22.065	21.769	8.575	1.00	17.39
2489	CA	ALA	A	344	22.809	20.531	8.651	1.00	18.18
2490	C	ALA	A	344	22.583	19.807	9.966	1.00	19.20
2491	O	ALA	A	344	22.784	18.593	10.077	1.00	20.60
2492	CB	ALA	A	344	24.297	20.832	8.466	1.00	18.23
2493	N	ALA	A	345	22.134	20.542	10.974	1.00	19.41
2494	CA	ALA	A	345	21.900	19.977	12.300	1.00	19.17
2495	C	ALA	A	345	21.211	18.626	12.284	1.00	19.03
2496	O	ALA	A	345	21.746	17.655	12.825	1.00	19.54
2497	CB	ALA	A	345	21.118	20.990	13.127	1.00	19.37
2498	N	GLY	A	346	20.031	18.481	11.700	1.00	19.05
2499	CA	GLY	A	346	19.302	17.240	11.616	1.00	18.25
2500	C	GLY	A	346	20.038	16.124	10.895	1.00	18.83
2501	O	GLY	A	346	19.819	14.936	11.171	1.00	18.01
2502	N	ALA	A	347	20.907	16.443	9.944	1.00	19.83

Figure 2-40

2521	OE1	GLU	A	349	20.333	17.684	16.369	1.00	36.57
2522	OE2	GLU	A	349	22.176	18.863	16.064	1.00	35.08
2523	N	SER	A	350	21.411	12.764	12.952	1.00	29.09
2524	CA	SER	A	350	20.905	11.481	12.516	1.00	28.77
2525	C	SER	A	350	22.049	10.458	12.529	1.00	29.04
2526	O	SER	A	350	21.839	9.297	12.841	1.00	29.05
2527	CB	SER	A	350	20.348	11.539	11.089	1.00	28.76
2528	OG	SER	A	350	19.043	12.076	11.069	1.00	28.97
2529	N	ILE	A	351	23.246	10.918	12.176	1.00	28.95
2530	CA	ILE	A	351	24.426	10.066	12.186	1.00	29.01
2531	C	ILE	A	351	24.801	9.724	13.627	1.00	29.32
2532	O	ILE	A	351	25.060	8.551	13.918	1.00	29.82
2533	CB	ILE	A	351	25.611	10.703	11.453	1.00	28.57
2534	CG1	ILE	A	351	25.423	10.556	9.941	1.00	28.77
2535	CG2	ILE	A	351	26.940	10.091	11.861	1.00	28.44
2536	CD1	ILE	A	351	26.265	11.488	9.099	1.00	28.88
2537	N	TYR	A	352	24.714	10.695	14.530	1.00	28.96
2538	CA	TYR	A	352	25.000	10.452	15.938	1.00	29.99
2539	C	TYR	A	352	24.004	9.479	16.562	1.00	30.75
2540	O	TYR	A	352	24.407	8.671	17.391	1.00	32.84
2541	CB	TYR	A	352	25.012	11.723	16.779	1.00	28.66
2542	CG	TYR	A	352	25.850	12.864	16.269	1.00	26.47
2543	CD1	TYR	A	352	25.545	14.168	16.639	1.00	26.55
2544	CD2	TYR	A	352	26.948	12.650	15.451	1.00	25.98
2545	CE1	TYR	A	352	26.313	15.236	16.196	1.00	26.27
2546	CE2	TYR	A	352	27.708	13.705	14.984	1.00	26.13
2547	CZ	TYR	A	352	27.385	14.991	15.359	1.00	25.70
2548	OH	TYR	A	352	28.157	16.019	14.896	1.00	25.41
2549	N	SER	A	353	22.744	9.528	16.167	1.00	31.38
2550	CA	SER	A	353	21.742	8.592	16.666	1.00	32.24
2551	C	SER	A	353	21.926	7.201	16.064	1.00	32.63
2552	O	SER	A	353	21.565	6.189	16.681	1.00	32.93
2553	CB	SER	A	353	20.337	9.125	16.385	1.00	32.06
2554	OG	SER	A	353	20.266	10.510	16.706	1.00	32.40
2555	N	ILE	A	354	22.497	7.136	14.866	1.00	31.79
2556	CA	ILE	A	354	22.761	5.860	14.218	1.00	31.51
2557	C	ILE	A	354	23.987	5.200	14.844	1.00	32.97
2558	O	ILE	A	354	23.951	4.012	15.168	1.00	33.27
2559	CB	ILE	A	354	22.935	6.018	12.703	1.00	29.87
2560	CG1	ILE	A	354	21.576	6.159	12.009	1.00	29.52
2561	CG2	ILE	A	354	23.698	4.848	12.116	1.00	30.35
2562	CD1	ILE	A	354	21.606	6.908	10.688	1.00	27.41
2563	N	LEU	A	355	25.055	5.970	15.066	1.00	33.53
2564	CA	LEU	A	355	26.290	5.432	15.639	1.00	33.26
2565	C	LEU	A	355	26.082	4.959	17.072	1.00	33.69
2566	O	LEU	A	355	26.622	3.935</			

Figure 2-41

2584	N	ARG	A	358	25.135	1.515	16.982	1.00	37.51
2585	CA	ARG	A	358	26.271	0.683	16.685	1.00	37.58
2586	C	ARG	A	358	27.129	0.376	17.910	1.00	38.26
2587	O	ARG	A	358	27.577	-0.751	18.097	1.00	39.24
2588	CB	ARG	A	358	27.197	1.380	15.656	1.00	37.33
2589	CG	ARG	A	358	28.337	0.451	15.242	1.00	37.76
2590	CD	ARG	A	358	29.272	1.085	14.228	1.00	37.44
2591	NE	ARG	A	358	30.034	2.160	14.848	1.00	38.18
2592	CZ	ARG	A	358	30.884	2.965	14.221	1.00	38.70
2593	NH1	ARG	A	358	31.108	2.831	12.917	1.00	38.32
2594	NH2	ARG	A	358	31.479	3.932	14.919	1.00	38.15
2595	N	ASP	A	359	27.448	1.410	18.670	1.00	37.94
2596	CA	ASP	A	359	28.406	1.368	19.746	1.00	37.27
2597	C	ASP	A	359	27.808	1.313	21.132	1.00	38.02
2598	O	ASP	A	359	28.521	1.217	22.136	1.00	37.65
2599	CB	ASP	A	359	29.231	2.675	19.670	1.00	36.75
2600	CG	ASP	A	359	30.238	2.668	18.549	1.00	36.38
2601	OD1	ASP	A	359	30.280	1.693	17.771	1.00	36.72
2602	OD2	ASP	A	359	30.991	3.661	18.460	1.00	36.33
2603	N	GLN	A	360	26.491	1.483	21.216	1.00	38.96
2604	CA	GLN	A	360	25.810	1.516	22.509	1.00	39.05
2605	C	GLN	A	360	26.538	2.465	23.461	1.00	39.38
2606	O	GLN	A	360	26.698	2.168	24.643	1.00	39.53
2607	CB	GLN	A	360	25.660	0.130	23.099	1.00	39.41
2608	CG	GLN	A	360	24.973	-0.898	22.217	1.00	39.76
2609	CD	GLN	A	360	23.466	-0.769	22.178	1.00	40.29
2610	OE1	GLN	A	360	22.782	-0.477	23.159	1.00	39.32
2611	NE2	GLN	A	360	22.893	-0.991	20.988	1.00	40.99
2612	N	ALA	A	361	26.886	3.644	22.959	1.00	39.00
2613	CA	ALA	A	361	27.461	4.728	23.751	1.00	38.72
2614	C	ALA	A	361	26.683	6.012	23.442	1.00	38.04
2615	O	ALA	A	361	26.357	6.270	22.275	1.00	38.26
2616	CB	ALA	A	361	28.937	4.883	23.455	1.00	38.95
2617	N	VAL	A	362	26.325	6.779	24.460	1.00	35.95
2618	CA	VAL	A	362	25.509	7.982	24.250	1.00	33.68
2619	C	VAL	A	362	26.293	9.242	24.568	1.00	32.65
2620	O	VAL	A	362	26.684	9.490	25.703	1.00	31.11
2621	CB	VAL	A	362	24.215	7.874	25.077	1.00	33.18
2622	CG1	VAL	A	362	23.575	9.209	25.387	1.00	32.96
2623	CG2	VAL	A	362	23.209	6.988	24.346	1.00	32.67
2624	N	PRO	A	363	26.535	10.050	23.534	1.00	32.66
2625	CA	PRO	A	363	27.283	11.285	23.645	1.00	31.67
2626	C	PRO	A	363	26.671	12.173	24.705	1.00	31.09
2627	O	PRO	A	363	25.449	12.194	24.869	1.00	32.64
2628	CB	PRO	A	363	27.199	11.941	22.285	1.00	32.07
2629	CG	PRO	A	363	26.641	10.940	21.360	1.00	32.96
2630	CD	PRO	A	363	26.096	9.789	22.139	1.00	32.89
2631	N	PRO	A	364	27.495	12.901	25.434	1.00	30.09
2632	CA	PRO	A	364	27.032	13.733	26.516	1.00	29.72
2633	C	PRO	A	364	26.553	15.120	26.123	1.00	29.59
2634	O	PRO	A	364	26.782	15.591	25.016	1.00	28.83
2635	CB	PRO	A	364	28.284	13.863	27.386	1.00	29.18
2636	CG	PRO	A	364	29.418	13.799	26.423	1.00	29.36
2637	CD	PRO	A	364	28.974	12.883	25.323	1.00	29.95
2638	N	THR	A	365	25.950	15.787	27.100	1.00	28.90
2639	CA	THR	A	365	25.536	17.166	27.039	1.00	29.34
2640	C	THR	A	365	26.515	17.969	27.909	1.00	29.33
2641	O	THR	A	365	26.271	18.122	29.106	1.00	28.44
2642	CB	THR	A	365	24.119	17.418	27.589	1.00	30.33
2643	OG1	THR	A	365	23.174	16.540	26.967	1.00	31.73
2644	CG2	THR	A	365	23.680	18.864	27.360	1.00	29.24
2645	N	ILE	A	366	27.654	18.366	27.362	1.00	29.73
2646	CA	ILE	A	366	28.650	19.040	28.203	1.00	30.00

Figure 2-42

2647	C	ILE	A	366	28.162	20.419	28.621	1.00	31.27
2648	O	ILE	A	366	27.219	20.981	28.067	1.00	30.39
2649	CB	ILE	A	366	30.025	19.120	27.528	1.00	29.07
2650	CG1	ILE	A	366	30.052	20.205	26.451	1.00	29.20
2651	CG2	ILE	A	366	30.405	17.769	26.927	1.00	27.75
2652	CD1	ILE	A	366	31.415	20.552	25.913	1.00	28.17
2653	N	ASN	A	367	28.785	20.975	29.652	1.00	32.72
2654	CA	ASN	A	367	28.511	22.285	30.190	1.00	34.91
2655	C	ASN	A	367	27.251	22.403	31.019	1.00	36.61
2656	O	ASN	A	367	26.871	23.504	31.450	1.00	36.20
2657	CB	ASN	A	367	28.483	23.311	29.038	1.00	35.89
2658	CG	ASN	A	367	29.871	23.565	28.480	1.00	36.26
2659	OD1	ASN	A	367	30.866	23.259	29.146	1.00	37.27
2660	ND2	ASN	A	367	29.952	24.113	27.279	1.00	35.83
2661	N	LEU	A	368	26.596	21.297	31.326	1.00	39.08
2662	CA	LEU	A	368	25.351	21.292	32.094	1.00	41.70
2663	C	LEU	A	368	25.647	21.267	33.592	1.00	44.25
2664	O	LEU	A	368	25.388	20.294	34.299	1.00	44.89
2665	CB	LEU	A	368	24.506	20.106	31.655	1.00	40.63
2666	CG	LEU	A	368	23.160	19.841	32.309	1.00	40.11
2667	CD1	LEU	A	368	22.287	21.085	32.347	1.00	40.15
2668	CD2	LEU	A	368	22.447	18.702	31.590	1.00	38.98
2669	N	ASP	A	369	26.196	22.375	34.085	1.00	46.52
2670	CA	ASP	A	369	26.643	22.493	35.460	1.00	48.49
2671	C	ASP	A	369	25.472	22.540	36.426	1.00	49.89
2672	O	ASP	A	369	25.518	21.893	37.476	1.00	50.35
2673	CB	ASP	A	369	27.544	23.715	35.641	1.00	48.44
2674	CG	ASP	A	369	28.783	23.682	34.769	1.00	48.89
2675	OD1	ASP	A	369	29.283	24.771	34.401	1.00	49.53
2676	OD2	ASP	A	369	29.284	22.587	34.435	1.00	48.33
2677	N	ASN	A	370	24.430	23.299	36.104	1.00	51.52
2678	CA	ASN	A	370	23.261	23.423	36.964	1.00	52.70
2679	C	ASN	A	370	21.951	23.438	36.185	1.00	53.77
2680	O	ASN	A	370	21.512	24.515	35.756	1.00	53.47
2681	CB	ASN	A	370	23.326	24.734	37.759	1.00	52.88
2682	CG	ASN	A	370	24.420	24.856	38.775	1.00	53.02
2683	OD1	ASN	A	370	25.288	25.726	38.676	1.00	52.97
2684	ND2	ASN	A	370	24.419	23.967	39.766	1.00	53.88
2685	N	PRO	A	371	21.289	22.302	36.046	1.00	55.26
2686	CA	PRO	A	371	20.009	22.231	35.356	1.00	57.50
2687	C	PRO	A	371	19.056	23.295	35.870	1.00	60.20
2688	O	PRO	A	371	19.124	23.621	37.064	1.00	61.29
2689	CB	PRO	A	371	19.481	20.849	35.667	1.00	56.46
2690	CG	PRO	A	371	20.611	20.064	36.190	1.00	56.02
2691	CD	PRO	A	371	21.728	20.992	36.542	1.00	55.51
2692	N	ASP	A	372	18.18				

Figure 2-43

2710	CA	GLY	A	374	12.019	21.821	36.531	1.00	71.79
2711	C	GLY	A	374	12.488	20.762	35.569	1.00	72.06
2712	O	GLY	A	374	11.663	19.944	35.116	1.00	72.74
2713	N	CYS	A	375	13.776	20.705	35.244	1.00	71.14
2714	CA	CYS	A	375	14.273	19.700	34.302	1.00	70.11
2715	C	CYS	A	375	14.845	18.495	35.029	1.00	69.27
2716	O	CYS	A	375	16.026	18.445	35.367	1.00	69.95
2717	CB	CYS	A	375	15.295	20.356	33.373	1.00	70.22
2718	SG	CYS	A	375	14.615	21.786	32.484	1.00	70.33
2719	N	ASP	A	376	14.003	17.492	35.257	1.00	67.38
2720	CA	ASP	A	376	14.353	16.293	35.989	1.00	65.40
2721	C	ASP	A	376	14.761	15.117	35.118	1.00	63.43
2722	O	ASP	A	376	14.848	13.977	35.602	1.00	63.21
2723	CB	ASP	A	376	13.144	15.872	36.851	1.00	66.52
2724	CG	ASP	A	376	11.940	15.452	36.031	1.00	67.35
2725	OD1	ASP	A	376	11.974	15.549	34.786	1.00	67.44
2726	OD2	ASP	A	376	10.925	15.017	36.628	1.00	67.75
2727	N	LEU	A	377	14.953	15.337	33.820	1.00	60.30
2728	CA	LEU	A	377	15.263	14.233	32.913	1.00	56.65
2729	C	LEU	A	377	16.745	13.893	32.912	1.00	54.35
2730	O	LEU	A	377	17.586	14.727	33.248	1.00	54.22
2731	CB	LEU	A	377	14.804	14.587	31.496	1.00	56.05
2732	CG	LEU	A	377	13.342	14.988	31.318	1.00	55.48
2733	CD1	LEU	A	377	13.151	15.780	30.034	1.00	55.31
2734	CD2	LEU	A	377	12.450	13.755	31.324	1.00	55.45
2735	N	ASP	A	378	17.072	12.669	32.518	1.00	51.50
2736	CA	ASP	A	378	18.466	12.246	32.405	1.00	49.45
2737	C	ASP	A	378	19.063	12.822	31.118	1.00	47.99
2738	O	ASP	A	378	18.941	12.271	30.023	1.00	47.05
2739	CB	ASP	A	378	18.579	10.724	32.418	1.00	49.34
2740	CG	ASP	A	378	19.988	10.196	32.572	1.00	48.74
2741	OD1	ASP	A	378	20.188	8.963	32.538	1.00	48.13
2742	OD2	ASP	A	378	20.931	11.003	32.733	1.00	49.41
2743	N	PHE	A	379	19.757	13.945	31.255	1.00	46.19
2744	CA	PHE	A	379	20.293	14.689	30.135	1.00	44.78
2745	C	PHE	A	379	21.708	14.267	29.762	1.00	44.38
2746	O	PHE	A	379	22.392	14.967	29.015	1.00	44.31
2747	CB	PHE	A	379	20.289	16.185	30.455	1.00	44.27
2748	CG	PHE	A	379	18.959	16.872	30.410	1.00	43.99
2749	CD1	PHE	A	379	18.592	17.747	31.419	1.00	43.84
2750	CD2	PHE	A	379	18.069	16.671	29.370	1.00	44.12
2751	CE1	PHE	A	379	17.374	18.397	31.397	1.00	43.77
2752	CE2	PHE	A	379	16.850	17.315	29.337	1.00	44.24
2753	CZ	PHE	A	379	16.497	18.184	30.358	1.00	43.96
2754	N	VAL	A	380	22.144	13.120	30.252	1.00	43.74
2755	CA	VAL	A	380	23.491	12.604	30.043	1.00	42.47
2756	C	VAL	A	380	24.485	13.738	30.306	1.00	42.16
2757	O	VAL	A	380	25.133	14.254	29.412	1.00	41.83
2758	CB	VAL	A	380	23.717	11.953	28.690	1.00	41.28
2759	CG1	VAL	A	380	25.002	11.135	28.721	1.00	40.26
2760	CG2	VAL	A	380	22.530	11.071	28.317	1.00	41.05
2761	N	PRO	A	381	24.545	14.148	31.578	1.00	42.27
2762	CA	PRO	A	381	25.180	15.367	31.990	1.00	42.11
2763	C	PRO	A	381	26.599	15.644	31.608	1.00	41.67
2764	O	PRO	A	381	26.806	16.781	31.118	1.00	43.27
2765	CB	PRO	A	381	25.021	15.391	33.511	1.00	42.44
2766	CG	PRO	A	381	23.830	14.555	33.781	1.00	42.72
2767	CD	PRO	A	381	23.743	13.541	32.680	1.00	42.38
2768	N	HIS	A	382	27.641	14.854	31.837	1.00	40.46
2769	CA	HIS	A	382	28.972	15.361	31.463	1.00	40.21
2770	C	HIS	A	382	29.808	14.418	30.635	1.00	41.00
2771	O	HIS	A	382	30.612	14.846	29.797	1.00	39.92
2772	CB	HIS	A	382	29.745	15.751	32.740	1.00	39.82

Figure 2-44

2773	CG	HIS	A	382	29.317	17.068	33.305	1.00	39.32
2774	ND1	HIS	A	382	29.629	18.266	32.705	1.00	39.09
2775	CD2	HIS	A	382	28.543	17.367	34.375	1.00	39.39
2776	CE1	HIS	A	382	29.086	19.250	33.393	1.00	39.48
2777	NE2	HIS	A	382	28.422	18.738	34.413	1.00	39.23
2778	N	GLU	A	383	29.706	13.118	30.916	1.00	42.14
2779	CA	GLU	A	383	30.521	12.126	30.227	1.00	43.32
2780	C	GLU	A	383	29.638	11.155	29.456	1.00	42.41
2781	O	GLU	A	383	28.503	10.903	29.847	1.00	41.73
2782	CB	GLU	A	383	31.403	11.362	31.220	1.00	45.87
2783	CG	GLU	A	383	32.071	12.198	32.299	1.00	48.56
2784	CD	GLU	A	383	33.412	12.759	31.859	1.00	50.99
2785	OE1	GLU	A	383	34.217	12.003	31.260	1.00	51.92
2786	OE2	GLU	A	383	33.672	13.962	32.105	1.00	52.07
2787	N	ALA	A	384	30.166	10.620	28.357	1.00	42.07
2788	CA	ALA	A	384	29.437	9.632	27.575	1.00	41.28
2789	C	ALA	A	384	28.935	8.511	28.488	1.00	41.42
2790	O	ALA	A	384	29.646	8.072	29.392	1.00	40.84
2791	CB	ALA	A	384	30.318	9.038	26.491	1.00	40.98
2792	N	ARG	A	385	27.719	8.050	28.221	1.00	41.17
2793	CA	ARG	A	385	27.134	6.969	28.987	1.00	41.16
2794	C	ARG	A	385	27.155	5.663	28.204	1.00	41.68
2795	O	ARG	A	385	26.740	5.612	27.048	1.00	43.05
2796	CB	ARG	A	385	25.688	7.287	29.379	1.00	41.25
2797	CG	ARG	A	385	25.008	6.145	30.128	1.00	41.15
2798	CD	ARG	A	385	24.890	6.475	31.606	1.00	40.96
2799	NE	ARG	A	385	23.866	7.495	31.831	1.00	41.21
2800	CZ	ARG	A	385	24.175	8.720	32.233	1.00	41.50
2801	NH1	ARG	A	385	25.455	9.016	32.428	1.00	41.34
2802	NH2	ARG	A	385	23.211	9.609	32.418	1.00	42.12
2803	N	GLN	A	386	27.568	4.596	28.867	1.00	41.57
2804	CA	GLN	A	386	27.548	3.262	28.264	1.00	40.47
2805	C	GLN	A	386	26.152	2.680	28.446	1.00	39.88
2806	O	GLN	A	386	25.497	2.999	29.451	1.00	39.50
2807	CB	GLN	A	386	28.622	2.417	28.935	1.00	41.01
2808	CG	GLN	A	386	28.533	0.926	28.674	1.00	40.91
2809	CD	GLN	A	386	29.158	0.575	27.341	1.00	41.24
2810	OE1	GLN	A	386	30.355	0.781	27.144	1.00	41.99
2811	NE2	GLN	A	386	28.338	0.075	26.430	1.00	41.97
2812	N	VAL	A	387	25.622	1.979	27.446	1.00	38.93
2813	CA	VAL	A	387	24.293	1.392	27.543	1.00	38.54
2814	C	VAL	A	387	24.315	-0.048	27.017	1.00	38.79
2815	O	VAL	A	387	25.250	-0.473	26.346	1.00	38.11
2816	CB	VAL	A	387	23.166	2.146	26.817	1.00	37.66
2817	CG1	VAL	A	387	22.938	3.547	27.358	1.00	36.33
2818									

Figure 2-45

2836	CE	MET	A	390	21.765	3.567	22.063	1.00	37.25
2837	N	GLU	A	391	17.620	-0.654	21.248	1.00	43.99
2838	CA	GLU	A	391	17.201	-1.001	19.892	1.00	46.08
2839	C	GLU	A	391	16.864	0.206	19.024	1.00	45.41
2840	O	GLU	A	391	17.167	0.247	17.826	1.00	44.59
2841	CB	GLU	A	391	16.005	-1.963	19.929	1.00	48.01
2842	CG	GLU	A	391	16.255	-3.301	20.576	1.00	51.25
2843	CD	GLU	A	391	16.345	-4.482	19.632	1.00	53.60
2844	OE1	GLU	A	391	15.617	-4.540	18.607	1.00	54.36
2845	OE2	GLU	A	391	17.166	-5.391	19.930	1.00	54.27
2846	N	TYR	A	392	16.214	1.215	19.591	1.00	44.78
2847	CA	TYR	A	392	15.787	2.388	18.871	1.00	44.24
2848	C	TYR	A	392	16.312	3.695	19.477	1.00	43.65
2849	O	TYR	A	392	16.257	3.870	20.701	1.00	43.45
2850	CB	TYR	A	392	14.257	2.501	18.881	1.00	44.89
2851	CG	TYR	A	392	13.475	1.323	18.387	1.00	45.69
2852	CD1	TYR	A	392	12.942	0.403	19.287	1.00	46.27
2853	CD2	TYR	A	392	13.246	1.120	17.032	1.00	45.96
2854	CE1	TYR	A	392	12.202	-0.678	18.851	1.00	46.79
2855	CE2	TYR	A	392	12.515	0.037	16.588	1.00	46.86
2856	CZ	TYR	A	392	11.991	-0.857	17.499	1.00	47.26
2857	OH	TYR	A	392	11.240	-1.930	17.071	1.00	47.84
2858	N	THR	A	393	16.527	4.677	18.599	1.00	41.43
2859	CA	THR	A	393	16.763	6.049	18.998	1.00	40.27
2860	C	THR	A	393	15.896	7.031	18.195	1.00	39.59
2861	O	THR	A	393	15.601	6.863	17.017	1.00	39.19
2862	CB	THR	A	393	18.227	6.496	18.876	1.00	40.35
2863	OG1	THR	A	393	18.792	6.069	17.624	1.00	40.81
2864	CG2	THR	A	393	19.062	5.964	20.019	1.00	39.93
2865	N	LEU	A	394	15.488	8.104	18.846	1.00	39.00
2866	CA	LEU	A	394	14.695	9.169	18.264	1.00	38.29
2867	C	LEU	A	394	15.567	10.401	18.030	1.00	37.46
2868	O	LEU	A	394	16.480	10.682	18.814	1.00	36.71
2869	CB	LEU	A	394	13.533	9.523	19.189	1.00	39.52
2870	CG	LEU	A	394	12.508	10.542	18.696	1.00	40.53
2871	CD1	LEU	A	394	11.158	9.876	18.456	1.00	40.54
2872	CD2	LEU	A	394	12.360	11.689	19.690	1.00	40.98
2873	N	CYS	A	395	15.300	11.120	16.940	1.00	36.66
2874	CA	CYS	A	395	16.095	12.310	16.628	1.00	35.56
2875	C	CYS	A	395	15.238	13.530	16.318	1.00	34.76
2876	O	CYS	A	395	14.505	13.532	15.328	1.00	34.93
2877	CB	CYS	A	395	17.014	12.019	15.441	1.00	34.91
2878	SG	CYS	A	395	17.954	13.469	14.915	1.00	35.28
2879	N	ASN	A	396	15.362	14.594	17.099	1.00	33.67
2880	CA	ASN	A	396	14.583	15.799	16.915	1.00	33.78
2881	C	ASN	A	396	15.283	16.976	16.256	1.00	32.51
2882	O	ASN	A	396	16.488	17.152	16.339	1.00	33.78
2883	CB	ASN	A	396	14.115	16.318	18.292	1.00	35.61
2884	CG	ASN	A	396	12.854	15.629	18.754	1.00	37.03
2885	OD1	ASN	A	396	12.208	14.917	17.979	1.00	36.89
2886	ND2	ASN	A	396	12.542	15.844	20.031	1.00	37.90
2887	N	SER	A	397	14.501	17.847	15.645	1.00	31.24
2888	CA	SER	A	397	14.937	19.065	14.990	1.00	30.08
2889	C	SER	A	397	13.728	19.999	14.871	1.00	29.36
2890	O	SER	A	397	12.686	19.517	14.403	1.00	28.86
2891	CB	SER	A	397	15.460	18.847	13.579	1.00	29.66
2892	OG	SER	A	397	16.795	18.440	13.514	1.00	30.44
2893	N	PHE	A	398	13.798	21.220	15.377	1.00	28.10
2894	CA	PHE	A	398	12.630	22.116	15.262	1.00	28.51
2895	C	PHE	A	398	13.071	23.370	14.525	1.00	28.82
2896	O	PHE	A	398	14.295	23.555	14.417	1.00	30.86
2897	CB	PHE	A	398	12.006	22.417	16.613	1.00	28.54
2898	CG	PHE	A	398	11.817	21.230	17.522	1.00	28.25

Figure 2-46

Figure 2-47

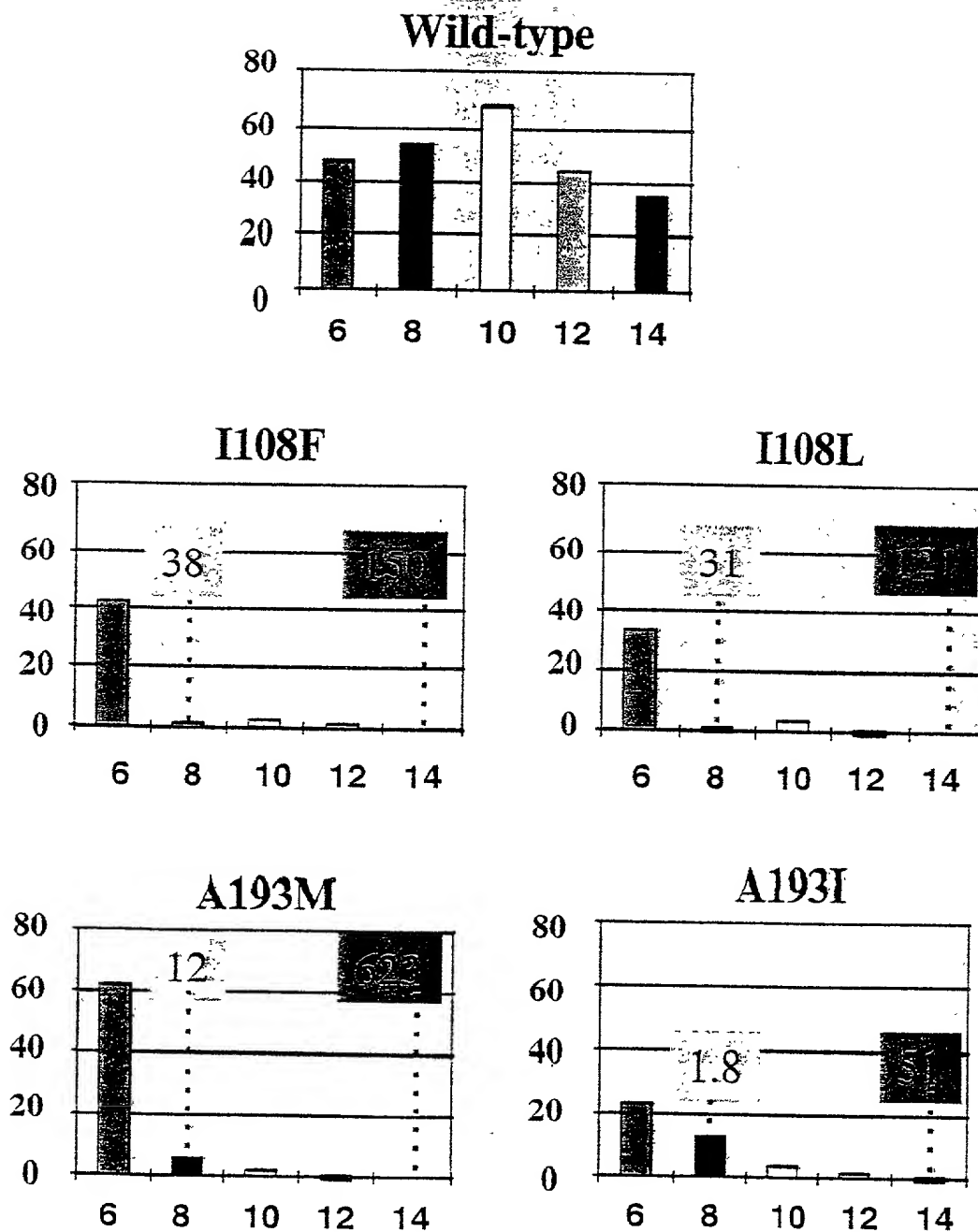
2962	C	ILE	A	408	14.199	5.975	13.852	1.00	32.25
2963	O	ILE	A	408	13.896	5.536	12.746	1.00	31.08
2964	CB	ILE	A	408	12.025	6.322	15.033	1.00	30.12
2965	CG1	ILE	A	408	11.353	7.157	16.132	1.00	29.79
2966	CG2	ILE	A	408	12.305	4.920	15.557	1.00	29.58
2967	CD1	ILE	A	408	9.895	6.798	16.326	1.00	29.42
2968	N	PHE	A	409	15.284	5.614	14.523	1.00	34.35
2969	CA	PHE	A	409	16.214	4.642	13.950	1.00	36.66
2970	C	PHE	A	409	16.134	3.342	14.724	1.00	38.51
2971	O	PHE	A	409	15.690	3.343	15.874	1.00	38.95
2972	CB	PHE	A	409	17.635	5.215	13.925	1.00	36.47
2973	CG	PHE	A	409	17.789	6.215	12.808	1.00	36.23
2974	CD1	PHE	A	409	17.643	7.567	13.065	1.00	36.49
2975	CD2	PHE	A	409	17.991	5.788	11.505	1.00	35.84
2976	CE1	PHE	A	409	17.755	8.487	12.036	1.00	36.42
2977	CE2	PHE	A	409	18.093	6.696	10.475	1.00	36.01
2978	CZ	PHE	A	409	17.977	8.051	10.745	1.00	36.45
2979	N	LYS	A	410	16.465	2.241	14.066	1.00	40.81
2980	CA	LYS	A	410	16.395	0.937	14.720	1.00	42.76
2981	C	LYS	A	410	17.648	0.123	14.412	1.00	43.74
2982	O	LYS	A	410	18.141	0.139	13.281	1.00	42.97
2983	CB	LYS	A	410	15.147	0.184	14.279	1.00	43.67
2984	CG	LYS	A	410	15.072	-1.261	14.749	1.00	45.15
2985	CD	LYS	A	410	13.842	-1.944	14.178	1.00	46.70
2986	CE	LYS	A	410	13.728	-3.393	14.600	1.00	47.69
2987	NZ	LYS	A	410	13.392	-3.506	16.051	1.00	48.43
2988	N	LYS	A	411	18.133	-0.567	15.439	1.00	45.19
2989	CA	LYS	A	411	19.314	-1.409	15.301	1.00	47.01
2990	C	LYS	A	411	18.931	-2.679	14.539	1.00	48.00
2991	O	LYS	A	411	17.858	-3.221	14.794	1.00	47.64
2992	CB	LYS	A	411	19.882	-1.782	16.661	1.00	47.51
2993	CG	LYS	A	411	21.236	-2.461	16.610	1.00	48.43
2994	CD	LYS	A	411	21.829	-2.606	18.008	1.00	49.25
2995	CE	LYS	A	411	21.660	-4.036	18.505	1.00	49.84
2996	NZ	LYS	A	411	22.313	-4.225	19.835	1.00	50.37
2997	N	ILE	A	412	19.767	-3.087	13.601	1.00	49.72
2998	CA	ILE	A	412	19.469	-4.274	12.799	1.00	51.86
2999	C	ILE	A	412	20.459	-5.392	13.085	1.00	52.16
3000	O	ILE	A	412	20.167	-6.540	12.754	1.00	52.95
3001	CB	ILE	A	412	19.422	-3.917	11.307	1.00	53.06
3002	CG1	ILE	A	412	18.129	-4.459	10.671	1.00	53.46
3003	CG2	ILE	A	412	20.640	-4.413	10.543	1.00	53.46
3004	CD1	ILE	A	412	17.892	-3.896	9.278	1.00	53.36
3005	OXT	ILE	A	412	21.521	-5.114	13.639	1.00	52.95
3006	ILE	A	412						
3007	C1	CER	A	413	16.270	27.008	14.939	1.00	42.62
3008	N1	CER	A	413	15.405	28.001	15.549	1.00	43.68
3009	O1	CER	A	413	16.728	30.271	11.664	1.00	41.32
3010	C2	CER	A	413	16.925	27.331	13.561	1.00	38.73
3011	O2	CER	A	413	16.493	25.921	15.481	1.00	43.30
3012	C3	CER	A	413	15.986	28.354	12.880	1.00	40.31
3013	O3	CER	A	413	14.813	27.662	12.446	1.00	40.48
3014	C4	CER	A	413	16.661	29.036	11.703	1.00	40.39
3015	C5	CER	A	413	17.226	28.267	10.507	1.00	40.11
3016	C6	CER	A	413	17.265	29.232	9.297	1.00	39.90
3017	C7	CER	A	413	18.711	29.652	9.103	1.00	40.02
3018	C8	CER	A	413	19.383	29.404	7.982	1.00	39.25
3019	C9	CER	A	413	20.833	29.912	7.969	1.00	39.77
3020	C10	CER	A	413	20.766	31.443	7.867	1.00	39.44
3021	C11	CER	A	413	21.590	32.160	8.641	1.00	39.99
3022	C12	CER	A	413	21.550	33.685	8.529	1.00	40.81
3023	O	HOH	501	21.907	17.399	19.574	1.00	18.60	O
3024	O	HOH	502	21.318	20.702	-2.438	1.00	24.78	O

Figure 2-48



KAS Assay Results

Specific Activity (pmol/min/ng)



Acyl-ACP Substrates

FIGURE 4

Comparison of the Decrease in Activity on 8:0 and 14:0 Compared to 6:0-ACP

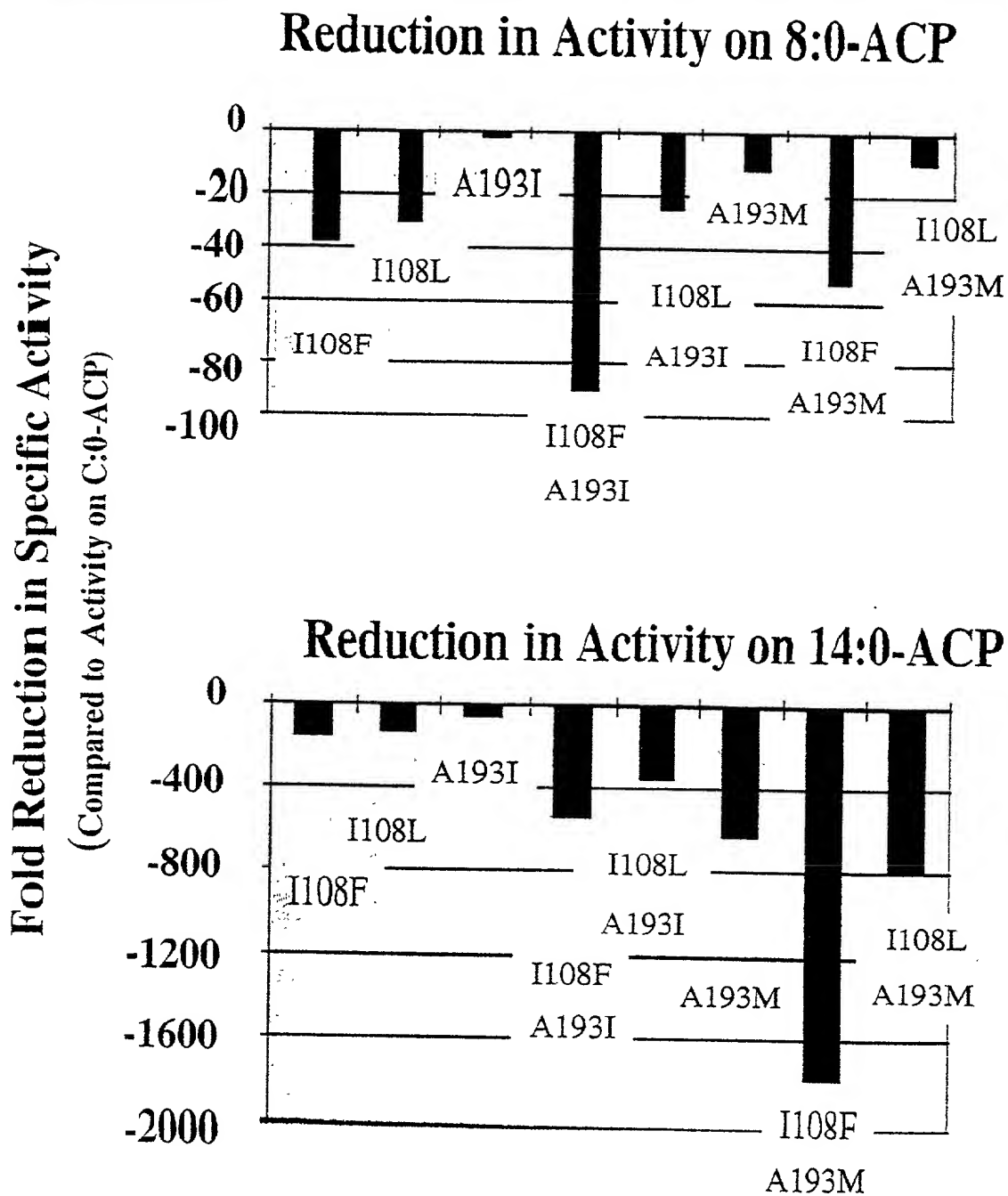


FIGURE 5

Comparison of the 6:0 Activity of the Single and Double Mutants

Specific Activity on 6:0-ACP

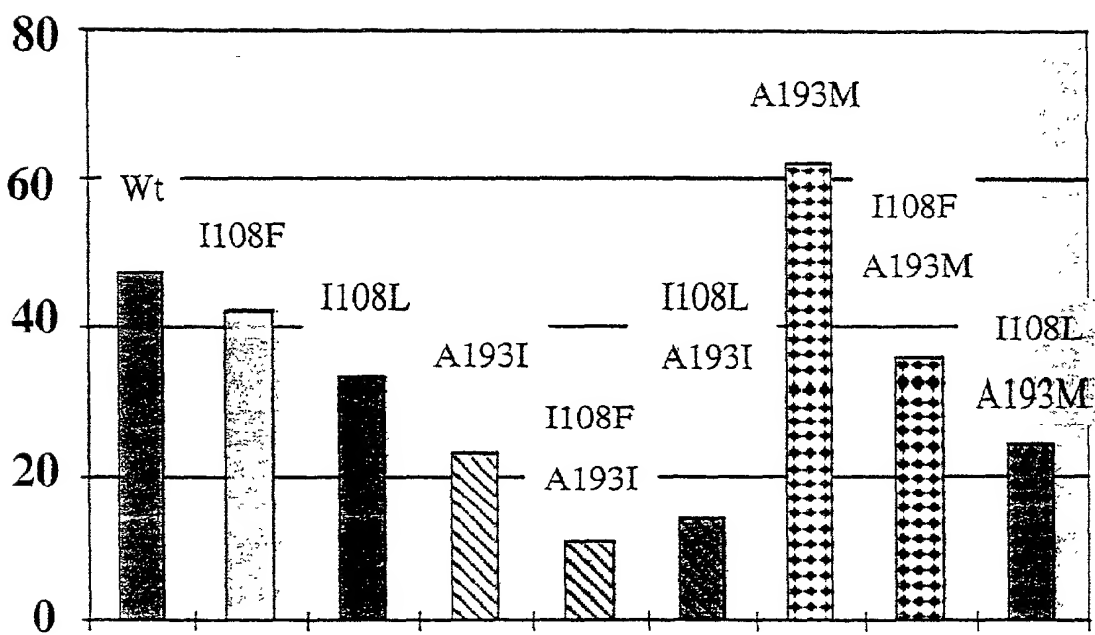


FIGURE 6

006050-62216560

Decreasing the Length	Increasing the Length
I108F	L111A
I108L	F133A
A193I	L111A, F133A
A193M	I108A, L111A, I114A
I108F, A193I	L197A
I108F, A193M	F133A, L197A
I108L, A193I	I108A, L111A, I114A, F133A, L197A
I108L, A193M	

Mutations Introduced into *E. coli* KAS II

FIGURE 7

006050* 6276560

Cpu KAS1 homodimer

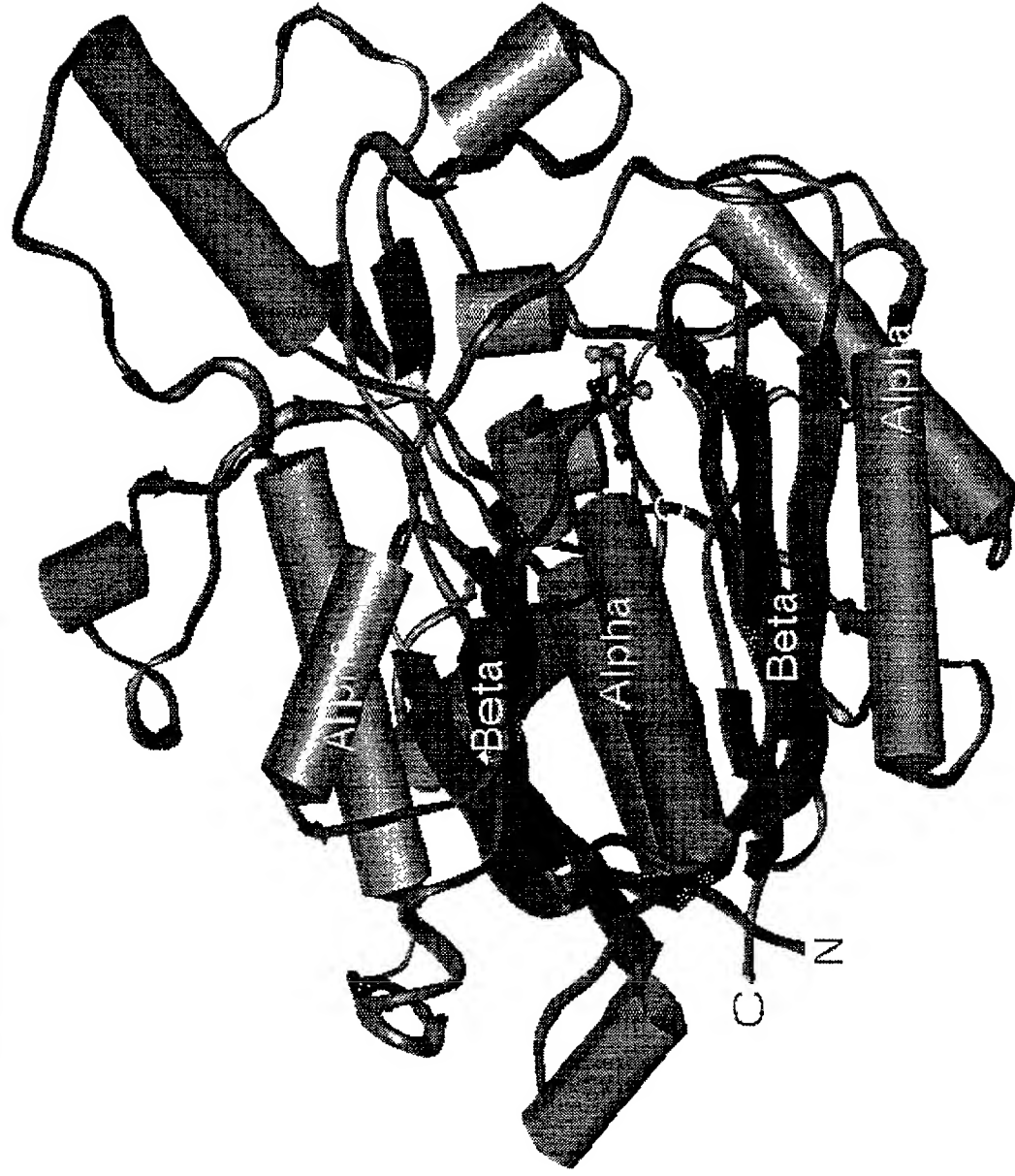


FIGURE 8

006090" 62216560

Cpu Kas IV

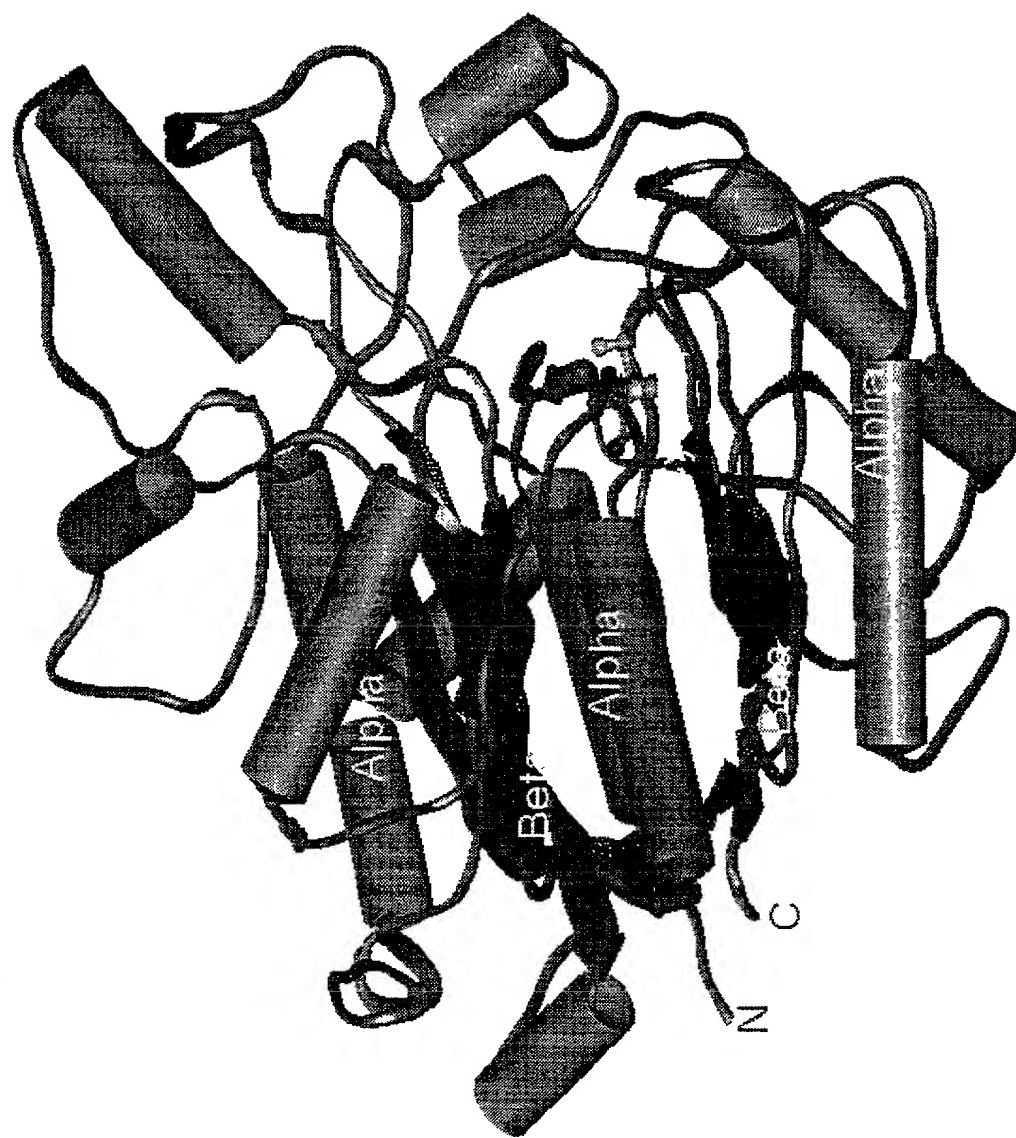


FIGURE 9

KAS I / KAS IV

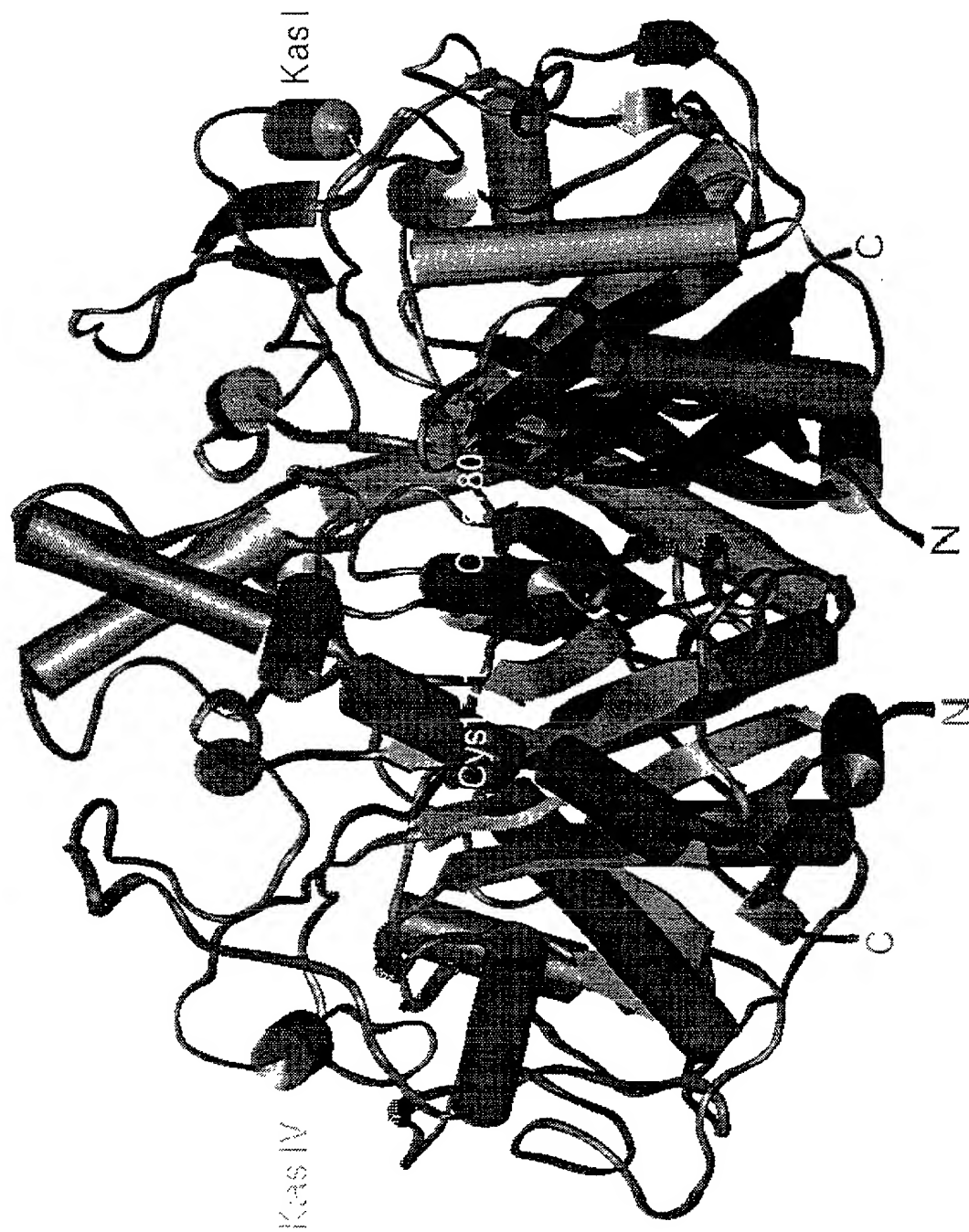


FIGURE 10

006090-6231550

<i>E.coli</i> Kas II	<i>C.pu</i> KAS IV
I108	M110
L111	M113
L113	V115
I114	F116
F133	C134
I138	T139
L197	I198
G203	V204

**Sequence Differences
in the Hydrophobic
Pockets of *E.coli* KAS II
and *C.pu* KAS IV**

Figure 11

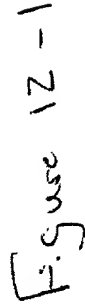


Figure 12-1

	370	380	390	400	410	420	430	440	450	460	470	480
LADAGVSPEDVNYINAHATSTPAGDLAEINAIKRV	-GQNS-ELKVNSTKSMIGHLLGAAAGGLEAIAIVKAI	/IHTPINLENP	DPGVLDLLVGNKK	EQHEVVKVAL								
At kasI .pro	LEDAGVSPEDVNYINAHATSTLAGDLAEINAIKVFF	---KSTVS-GIKINATKSMIGHCLGAAAGGLEAIAIVKAI	INIGWLHPSINQFNP	---EQAVDFDI-VPNEK	---KQHEVDVAI	411						
Br kas 50 .pro	LEDAGVSPEDVNYINAHATSTLAGDLAEINAIKVFF	---KSTVS-GIKINATKSMIGHCLGAAAGGLEAIAIVKAI	INIGWLHPSINQFNP	---EPAVDFDI-VANEK	---KQHEVNVAI	409						
Ch kas I .pro	LEDAGVSPEDVNYINAHATSTLAGDLAEINAIKVFF	---KNVK-DIKINATKSMIGHCLGASGGLEAIAITK	INGITGWLHPSINQFNP	---EPSVEFDI-VANKK	---QQHEVNVAI	330						
Ch kas I -1 .pro	LEDAGVSPEDVNYINAHATSTLAGDLAEINAIKVFF	---KNVK-EITINATKSMIGHCLGASGGLEAIAITK	IGITGWLHPSINQFNP	---EPSVEFDI-VANKK	---QQHEVNVAI	421						
Cpu kas I .pro	LEDAGVSPEDVNYINAHATSTLAGDLAEINAIKVFF	---KNVK-DIKINATKSMIGHCLGASGGLEAIAITK	INGITGWLHPSINQFNP	---EPSVEFDI-VANKK	---QQHEVNVAI	410						
cpu kas I -1 .pro	LEDAGVSPEDVNYINAHATSTLAGDLAEINAIKVFF	---KNVK-EIKINATKSMIGHCLGASGGLEAIAITK	IGITGWLHPSINQFNP	---EPSVEFDI-VANKK	---QQHEVNVAI	408						
Hv kas 12 .pro	LRDAGVAPEDVNYINAHATSTLAGDLAEVRAIKVFF	---KNPS-EIKINATKSMIGHCLGAAAGGLEAIAITK	ISITGWLHPTINQFNP	---EPEVDFDI-VANEK	---KQHEVNVGI	407						
Rc kas 50 .pro	LEDAGVSPEDVNYINAHATSTLAGDLAEINAIKVFF	---KNVS-DIKINATKSMIGHCLGAAAGGLEAIAITK	ITGWLHPTINQFNP	---EPSVEFDI-VANKK	---QQHEVNVAI	409						
Cc kas .pro	LVDAGVSPEDVNYINAHATSTLAGDLAEVNAIKVFF	---KDTSEIKMNGTKSMIGHCLGASGGLEAIAITK	ITGWLHPTINQYDL	---EPQVTIDI-VPNVK	---KQHEVNVGI	400						
Ch kas IV-1 .pro	LAQSGVSREDVNYINAHATSTPAGDIKEYQALHCF	---GQNN-ELKVNSTKSMIGHLLGAAAGGLEAIAIVVQA	IRIGWIHPNINLENP	---DEGVDTKLLVGPKK	---ERLNIKUGL	401						
Ch kas IV .pro	LAQSGVSREDVNYINAHATSTPAGDIKEYQALHCF	---GQNS-ELRVNSTKSMIGHLLGAGGVEAVAVVQA	IRIGWIHPNINLEDP	---DEGVDAKLLVGPKK	---EKLKVKUGL	401						
Cpu kas IV .pro	LAQSGVSREDVNYINAHATSTPAGDIKEYQALHCF	---GQNR-ELKVNSTKSMIGHLLGAAAGGLEAIAIVVQA	IRIGWIHPNINLENP	---DEGVDTKLLVGPKK	---ERLNIKUGL	401						
Cw kas A -1 .pro	LAQSGVSKEDVNYINAHATSTPAGDIKEYQALHCF	---GQNS-ELRVNSTKSMIGHLLGAAAGGLEAIAIVVQA	IRIGWIHPNINLEDP	---DKAVDAKLLVGPKK	---ERLNIKUGL	401						
Cw kas A -2 .pro	LAQSGVSKEDVNYINAHATSTPAGDIKEYQALHCF	---SQNS-ELRVNSTKSMIGHLLGAAAGGLEAIAIVVQA	IRIGWIHPNINLENP	---DDGVDAKLLVGPKK	---ERLNIKUGL	401						
Hv kas ORF22 (kas	IV LADSGVAREEINYNNAHATSTQSGDLKEYEAIVRCF	---GQNP-QLRVNSTKSMIGHLLGAAAGGLEAIAITQA	IRIGWIHPNINLENP	---EKVVDVGLVVGSEK	---ERCEVVKVAL	401						
Hv kas ORF25 (kas	IV LADAGVTRQDINYNNAHATSTQLGDLKEFEALRRCF	---GQNP-QLRVNSTKSMIGHLLGAAAGGLEAIAITQA	IRIGWIHPNINLENP	---EKVVDVGLVVGSEK	---ERCEVVKVAL	401						
Rc kas 46 .pro	LARSGVSKEDVNYINAHATSTPAGDLKEYEALMRCF	---SQNP-DLRVNSTKSMIGHLLGAAAGGLEAIAITQA	IRIGWIHPNINLENP	---EEGVDTKLLVGPKK	---ERLNIKUGL	401						
Ce kas .pro	IGNAHLEPKDIGVYNAHATSTPNGDSVEAEAV-RQVFP	EQNTA-----VSSVKGHIGHLLGAAAGGLEAIAITQA	IRIGWIHPNINLENP	---ETDEGNGLNLLRENQKWS	SDVSGNKSRSI	395						
CEM .pro	LKMARLEPTDQDVYNAHATSTLLGDKAECLAVASALLP	ORSKSKPLVTSNNKGAIGHLLGAAAGGLEAIAITQA	IRIGWIHPNINLENP	---ETDEGNGLNLLRENQKWS	SDVSGNKSRSI	421						
Ec kas II .pro	LRDAGIEASQIGVYNAHATSTPAGDKAEQAQVKTIF	---GEAASRVLVSTKSMIGHLLGAAAGGLEAIAITQA	IRIGWIHPNINLENP	---DEGCDDLPVPHEAR	---QVSGMEVTL	395						
Ec kas I .pro	MHGVDTP---IDYLNHSGTSTPVGVDVKELAAIREVF	---GDKS--PAISATKAMTGHSLGAAAGGLEAIAITQA	IRIGWIHPNINLENP	---DEQAA-GINI	VTET---TDRELITVVM	386						
M.tub.KasA .pro	LELAGLSPADIDHVNNAHATGTPVGDVLAEGRAINNAL	---GCIQ--AAVYAPKSAIGHSTGAVGALSVLVTIR	DGVIPTTLNYETP	---DPEIDLDDVWAGEPR	---YG-DYRVAV	398						
M.tub.KasB .pro	IQLAGLAPGDIHVNNAHATGTVQVGDVLAEGRAINNAL	---GQNR--PAVYAPKSAIGHSTGAVGALSVLVTIR	DGVIPTTLNYETP	---DPEIDLDDVWAGEPR	---PG-NYRVAI	420						
Rat . kas .pro	YQPGGVAPESLEYIEAHGTGTVQVGDVLAEGRAINNAL	---LIGSTKSNMGHPEPASGLAALTKVLLSLENGVW	APNLFHNP-NPEI	PALLDGRQVVDPR	---LPVRGGIVGI	399						
RtNode . pro	LADAELNPDDVDYINAHGTGTVANDEMETAIAIKRVF	---GDHAFQMSVSTKSMHAHCLGAAAGGLEAIAITQA	IRIGWIHPNINLENP	---DPQCDLDDVWAGEPR	---EQR-C-GSM	383						
Streppolyk .pro	LDEARRDPDSDVDYINAHGTATKQNDRHETSAFKRSL	---GEHAYRVPISSIKSMIGHSLGAVGSLEVAAT	ALAVEYGIPTTANLHDP	---DPELDDVWAGEPR	---EKR-VRHAI	399						
SYN kas .pro	LKDSGLKPEWVSYINAHGTSTPANDVTETRAIKQAL	---GNHAYNTIAVSTKSMIGHLLGSGGIEAVAT	VMAIAEDKVPTTINLENP	---DPECDLDDVWAGEPR	---ALI-VDVAL	397						
V .pro	IADAGITADKVGVYNAHGTSTPAGDKAETAIAVKSVEF	---GEHAYTLAVSTKSMIGHLLGAAAGGLEAIAITQA	IRIGWIHPNINLENP	---SEGCDDLVWAGEPR	---PVN-MEVAL	422						

Figure 12-4



SNSFGFGGHNSVAFAPFK--

490 500

At KAS I.pro	SNSFGFGGHNSVAFAPFK-P	431
Br Kas 50.pro	SNSFGFGGHNSVAFAPFK-P	429
Ch KAS I .pro	SNSFGFGGHNSVAFAPFK-P	350
Ch KAS I-1.pro	SNSFGFGGHNSVAFAPFK-P	441
Cpu KAS I.PRO	SNSFGFGGHNSVAFAPFK-P	430
cpuKAS I-1.PRO	SNSFGFGGHNSVAFAPFK-P	428
Hv Kas12.pro	SNSFGFGGHNSVVFAPFK-P	427
RcKas50.pro	SNSFGFGGHNSVAFAPFK	428
Cc Kas.pro	SNSFGFGGHNSVVFAPYK-P	420
Ch KAS IV-1.pro	SNSFGFGGHNSILFAPY--N	420
Ch KAS IV.pro	SNSFGFGGHNSILFAPCN	420
Cpu KAS IV.pro	SNSFGFGGHNSILFAPY--I	420
Cw KASA-1.pro	SNSFGFGGHNSILFAPCN-V	421
Cw Kasa-2.pro	SNSFGFGGHNSILFAPCN	420
Hv KasORF22(KAS I\	SNSFGFGGHNSILFAPFK	420
Hv KasORF25(KAS I\	SNSFGFGGHNSILFAPF	419
RcKas46.pro	SNSFGFGGHNSIIFAPYK	420
Ce.KAS.PRO	CNSFGFGATNASLILKQF.	414
CEM.pro	CNSFGFGGWNTSILFKWEGS	442
Ec KAS II.pro	CNSFGFGGTNGSLIF	410
Ec Kasi.pro	SNSFGFGGTNATLVMRKLK-D	406
M.tub.KasA.pro	NNSFGFGGHNVAFAGRY	416
M.tub.KasB.PRO	NNSFGFGGHNVAFAGRY	438
Rat. Kas.PRO	-NSFGFGGANVHVLQP-NAS	418
RtNode.pro	SNAFAMGGTNAVLAFRQV	401
StrepPolyk.pro	TVGSGFGGFSAMLLSRLE-R	419
SYN KAS.pro	SNSFGFGGHNVTLAFKKYQ	416
V.pro	SNSFGFGGTNGSILFKKAD	441

Figure 12-5

00004E00 060900

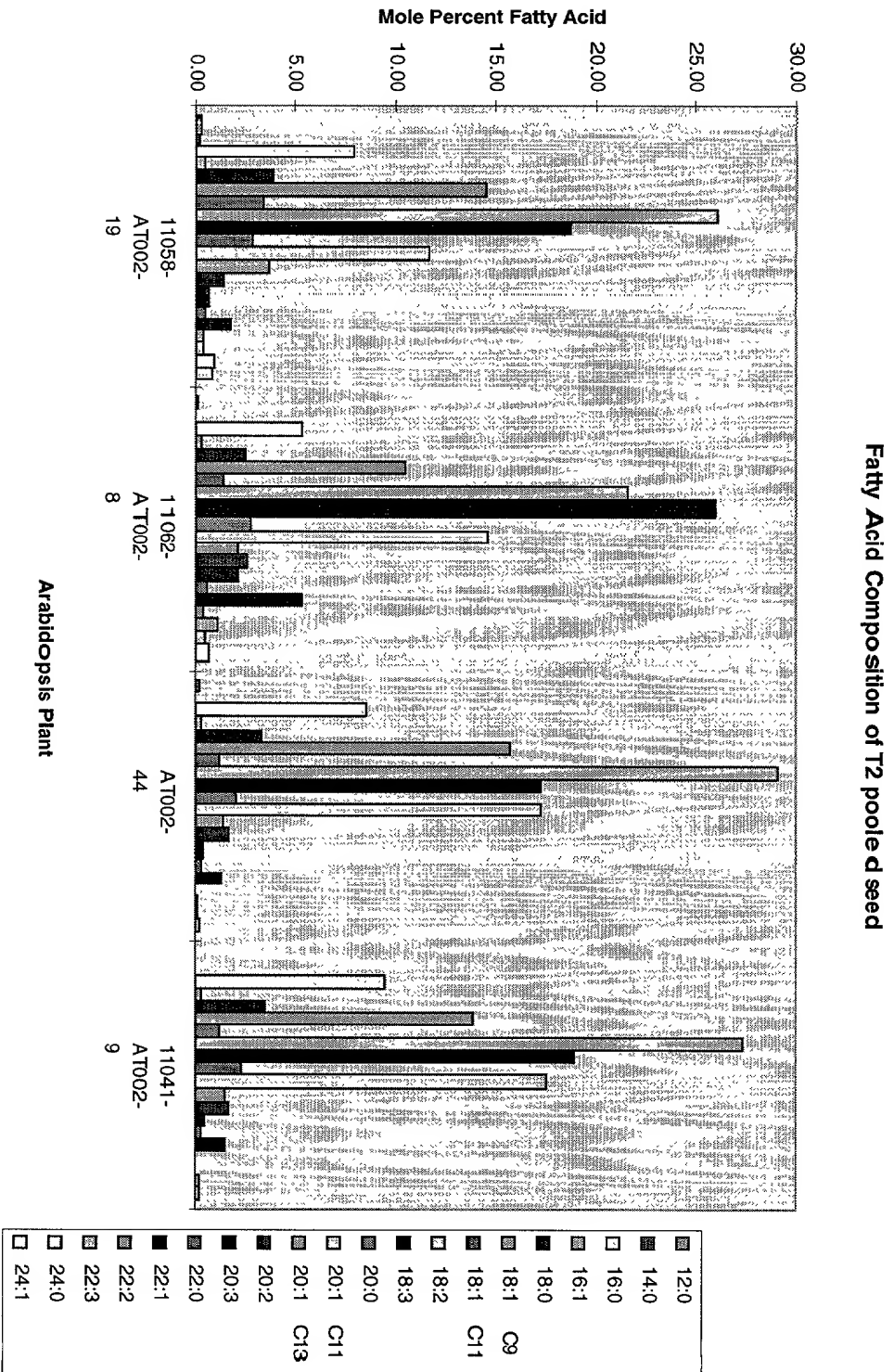


Figure 13

[illegible][illegible]

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25	26	27	28	29	30	31	32	33	34	35	36	37	38	39	40	41	42	43	44	45	46	47	48	49	50	51	52	53	54	55	56	57	58	59	60	61	62	63	64	65	66	67	68	69	70	71	72	73	74	75	76	77	78	79	80	81	82	83	84	85	86	87	88	89	90	91	92	93	94	95	96	97	98	99	100
1	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25	26	27	28	29	30	31	32	33	34	35	36	37	38	39	40	41	42	43	44	45	46	47	48	49	50	51	52	53	54	55	56	57	58	59	60	61	62	63	64	65	66	67	68	69	70	71	72	73	74	75	76	77	78	79	80	81	82	83	84	85	86	87	88	89	90	91	92	93	94	95	96	97	98	99	100